



ReaxFF Manual

Amsterdam Modeling Suite 2020

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ReaxFF is an engine for modeling chemical reactions with atomistic potentials based on the reactive force field approach developed by Prof. Adri van Duin and coworkers. SCM has modernized, parallelized and greatly optimized the original ReaxFF program.

1.1 What's new in ReaxFF 2020

ReaxFF is available in the [AMS driver](#) as one of the engines, which means that all *tasks that can be performed with the AMS driver* (page 9) are also available for ReaxFF. However, not all tasks from the classic ReaxFF standalone program are available in the ReaxFF AMS engine, so in the 2020 release of the Amsterdam Modeling Suite, the standalone ReaxFF program and the ReaxFF engine coexist. **The graphical user interface program AMSinput only sets up ReaxFF jobs as an engine to the AMS driver.**

For more information, see *ReaxFF Engine Features Vs. Old Standalone Program* (page 13).

Other new features:

- 0D, 1D, and 2D periodicity
- *Tapered bond orders* (page 3)
- *Charge constraints* (page 7)

Note: Development of the [old standalone ReaxFF program](#) has stopped.

REAXFF INPUT

This section describes the input keywords to the ReaxFF AMS engine.

See also:

- *AMS driver's tasks and properties* (page 9)

2.1 Force field specification

The only input key required by the engine is `ForceField`, used to select the *force field file* (page 45). Force fields *included in the Amsterdam Modeling Suite* (page 17) can be easily accessed using their file name, such as `CHO.ff`.

ForceField

Type String

Description Path to the force field parameter file. Absolute path if starting with `/` or `./`, relative to `$AMSRESOURCES/ForceFields/ReaxFF` otherwise.

2.2 Recommended lattice convention

The ReaxFF engine supports molecular (free boundary), 1D-, 2D-, and 3D-periodic systems. Non-orthorhombic lattices are supported in an arbitrary orientation. However, the engine is slightly more computationally efficient when the cell is oriented according to the convention used in standalone ReaxFF, i.e. lattice vector `c` aligned with the `z` axis and vector `b` in the `yz` plane (zero `x` component). The `Lattice` block in the *system definition* then looks like this:

```
System
  Lattice
    xx xy xz
      0 yy yz
      0 0 zz
  End
End
```

2.3 Smoothened potential energy surface

The keywords below can be used to enable the **tapered bond orders** and/or **improved torsion angle potentials**. Although the original ReaxFF torsion potential is the default to preserve backward compatibility, the corrected potentials eliminate energy discontinuities and work well with existing force fields.

Using the tapered bond order (the `TaperBO` key) does not change the potential form at the chemically relevant distances so it can be used with any force-field. It may improve the energy conservation during MD and make geometry optimizations with ReaxFF converge to much tighter criteria. The discontinuity and the correction for it are described in detail in *J. Phys. Chem. Lett.* 10 (2019) 7215 (<https://doi.org/10.1021/acs.jpcllett.9b02810>).

TaperBO

Type Bool

Default value No

GUI name Taper bond orders

Description Use tapered bond orders by Furman & Wales (DOI: 10.1021/acs.jpcllett.9b02810).

The discontinuity at small bond orders in the expression for torsion angles and conjugation contributions can alternatively be corrected for using the `Torsions 2013` correction. The corresponding terms are given by f_{10} (eq. 10b) and f_{12} (eq. 11b) in the [original ReaxFF paper](https://doi.org/10.1021/jp004368u) (<https://doi.org/10.1021/jp004368u>). The new expression for each term in f_{10} is $(1 - e^{-2\lambda_{23}BO^2})$ and in f_{12} the new expression is $\sin(\frac{\pi}{3}BO)^4$. The new expressions ensure correct asymptotic behavior for the $\frac{dE}{dBO}$ for $BO \rightarrow 0$.

Another discontinuity in the torsion angle term is when one or both valence angles approach 180 degrees. It is described in detail in *J. Chem. Phys.* 153 (2020) 021102 (<https://doi.org/10.1063/5.0013906>), and can be enabled with `FurmanTorsions Yes`.

See also:

Geometry optimization issues (page 51)

Torsions

Type Multiple Choice

Default value Original

Options [Original, 2013]

Description Version of the torsion potential expression.

FurmanTorsions

Type Bool

Default value No

Description Use $(\sin(\Theta_{ijk})\sin(\Theta_{jkl}))^3$ instead of $\sin(\Theta_{ijk})\sin(\Theta_{jkl})$ in the torsion energy term to remove discontinuity in the corresponding force.

2.4 Bond order and distance cutoffs

BondDistanceCutoff

Type Float

Default value 5.0

Unit Angstrom

Description Maximum distance between two atoms to be considered when searching for possible bonds.

BondOrderCutoff

Type Float

Default value 0.001

Description Minimum bond order required for a bond to be considered during the evaluation of the potential.

StrongBondCutoff

Type Float

Default value 0.3

Description Minimum bond order required for a bond to be returned to the driver for bonding analysis and molecule detection. Bonds below this threshold are only used to evaluate the potential and not written to result files.

2.5 Non-reactive mode

The engine can also be switched to a special non-reactive mode useful mainly for initial preparation of molecular dynamics simulations. This mode greatly reduces the occurrence of unwanted reactions when starting from an unrelaxed geometry. In these situations, we recommend running a short simulation with the `NonReactive` key to relieve the initial conformational strain and then restarting the MD run without this key.

Note that if you want to resume or extend an interrupted `NonReactive` run, it is recommended to also use the `EngineRestart` AMS key to supply the last ReaxFF `.rkf` file from the previous run. This enables the engine to load the bonding topology used during the previous run and ensure that the simulation is seamlessly restarted. If the `EngineRestart` key is not used, bonds will be re-detected in the first step and then preserved during the rest of the simulation.

NonReactive

Type Bool

Default value No

GUI name Non-reactive

Description Enable the non-reactive mode. Bonds are determined only once at the beginning and subsequent steps only update their bond orders. Thus, no new bonds can form during the simulation, but existing bonds can still stretch and dissociate.

2.6 Charge equilibration

Details of the charge equilibration (electronegativity equalization method, EEM) procedure can be adjusted using the `Charges` block.

```
Charges
  Constraint
    Charge float
    Region string
  End
  Converge
    Charge float
  End
  DisableChecks Yes/No
  Predictor
    Method [None | Simple]
```

(continues on next page)

```
End
  Solver [Direct | CG | MINRESQLP | SparseCG | None]
End
```

Charges

Type Block

Description Settings for the polarizable charge model.

Constraint

Type Block

Recurring True

Description Constrain the net charge of a given region.

Charge

Type Float

Default value 0.0

Description Desired net charge of the region.

Region

Type String

Description Name of the region to be constrained.

Converge

Type Block

Description Controls the convergence criteria for charge equilibration.

Charge

Type Float

Default value 1e-06

Description Requested upper bound on the sum of squared charge residuals.

DisableChecks

Type Bool

Default value No

Description Disable checks for suspicious or unphysical charges.

Predictor

Type Block

Description Settings for the prediction of new charges before running the solver.

Method

Type Multiple Choice

Default value Simple

Options [None, Simple]

Description Method used to predict the charges.

Solver**Type** Multiple Choice**Default value** SparseCG**Options** [Direct, CG, MINRESQLP, SparseCG, None]**Description** Algorithm used to solve the charge equilibration equations.

2.6.1 Charge constraints

The net charge of an arbitrary group of atoms can be constrained to a particular value using the `Constraint` block. This block can be repeated as needed to constrain multiple non-overlapping parts of the system. To define charge constraints, first define appropriate `regions`, in the `System` block and then set the `Region` key inside each `Constraint` block accordingly.

Note: Unlike the similar `MOLCHARGE` constraints in standalone ReaxFF, it is not necessary for the constrained regions to span a consecutive range of atoms. It is also not necessary to define constraints for all atoms in the system. The necessary sum of charges of any unconstrained atoms will be determined from the overall net charge of the entire system, as set by the `Charge` key in the `System` block.

In the following example, we constrain the net charge of one water molecule in a dimer while the other molecule automatically assumes the opposite charge to keep the whole system neutral:

```
System
  Charge 0.0
  Atoms
    O -0.0509 -0.2754 0.6371 region=donor
    H 0.0157 0.5063 0.0531 region=donor
    H -0.0055 -1.0411 0.0658 region=donor
    O 0.0981 1.7960 -1.2550 region=acceptor
    H -0.6686 2.2908 -1.5343 region=acceptor
    H 0.8128 2.3488 -1.5619 region=acceptor
  End
End

Engine ReaxFF
  ForceField Water2017.ff
  Charges
    Constraint Region=donor Charge=0.1
    # The following constraint is implied and need not be specified explicitly.
    # It is only shown here as an example of multiple constraints in a single_
↪system.
    Constraint Region=acceptor Charge=-0.1
  End
EndEngine
```


AMS DRIVER'S TASKS AND PROPERTIES

ReaxFF is an [engine](#) used by the AMS driver. While ReaxFF's specific options and properties are described in this manual, the definition of the system, the selection of the task and certain (PES-related) properties are documented in the AMS driver's manual.

In this page you will find useful links to the relevant sections of the [AMS driver's Manual](#).

3.1 Geometry, System definition

The definition of the system, i.e. the atom types and atomic coordinates (and optionally, the systems' net charge, the lattice vector, atomic masses for isotopes) are part of the AMS driver input. See the [System definition section of the AMS manual](#).

3.2 Tasks: exploring the PES

The job of the AMS driver is to handle all changes in the simulated system's geometry, e.g. during a geometry optimization or molecular dynamics calculation, using energy and forces calculated by the engine.

These are the tasks available in the AMS driver:

- [Single Point](#)
- [Geometry Optimization](#)
- [Transition State Search](#)
- [IRC \(Intrinsic Reaction Coordinate\)](#)
- [PESScan \(Potential Energy Surface Scan, including linear transit\)](#)
- [NEB \(Nudged Elastic Band\)](#)
- [Vibrational Analysis](#)
- [Molecular Dynamics](#)
- [GCMC \(Grand Canonical Monte Carlo\)](#)

3.3 Properties in the AMS driver

The following properties can be requested to the ReaxFF engine in the AMS driver's input:

- [Bond orders](#)

- Atomic charges
- Elastic tensor
- Nuclear Gradients / Forces
- Hessian
- Thermodynamic properties
- PES point character
- Phonons
- Stress tensor
- Elastic tensor

EREAXFF, ACKS2, LG DISPERSION

Note: Only the *ReaxFF force fields* (page 17) that mention eReaxFF and ACKS2 support those features. The LG dispersion correction is only implemented by force fields in the `dispersion` subdirectory.

4.1 eReaxFF: classical treatment of the explicit electron

eReaxFF calculations treat one or more electrons or holes explicitly¹.

An eReaxFF calculation **requires the following additional force-field parameters to be defined** (equation numbers are referring to the eReaxFF paper¹):

- The header of the force-field file must begin with the “[ereaxff acks2]” string,
- General parameter 27: the currently reserved p_{elho} parameter in the unpublished electron-hole interaction equation (which is still highly experimental and is subject to change),
- General parameter 37: the Gauss exponent parameter p_{val} describing the free electron, Eq(3),
- General parameter 41: a different taper radius for electron and hole interactions can be specified here,
- Atomic parameter 24: the α parameter in Eq(2),
- Atomic parameter 27: the β parameter in Eq(2),
- Atomic parameter 13: the p_{ij}^{xel2} parameter in Eq(4d),
- Bond parameter 16: the p_{ij}^{xel1} parameter in Eq(4d).

Additionally, since the eReaxFF method is usually coupled to the *ACKS2 charge equilibration method* (page 11), the ACKS2-related parameters should also be defined.

In the input geometry file, the explicit electrons are called E1 and the holes are called Eh.

The eReaxFF implementation is considered experimental, so users are advised to contact Adri van Duin regarding its use.

4.2 ACKS2 charge equilibration

The ACKS2 charge equilibration scheme has been implemented following the original paper².

¹ M. M. Islam et al., *eReaxFF: A Pseudoclassical Treatment of Explicit Electrons within Reactive Force Field Simulations*. J. Chem. Theory Comput. 12, 3463 (2016) <https://doi.org/10.1021/acs.jctc.6b00432>

² T. Verstraelen et al. *ACKS2: Atom-condensed Kohn-Sham DFT approximated to second order*. J. Chem. Phys. 138 (2013) 074108. <https://doi.org/10.1063/1.4791569>

Using the **ACKS2** scheme requires a suitable force-field, which is recognized by “[acks2]” at the start of the first line of force field file (note: the spaces around “acks2” are important!).

In addition to the general EEM parameters the ACKS2 scheme needs the general force-field parameter #35 (“Xamp”) and the atomic cut-off parameter #23 (“softcut”).

4.3 LG dispersion correction

The LG dispersion correction was implemented following the paper Liu et al.³

The LG dispersion correction is turned on when using a suitable forcefield, which is recognized by the “[lgDispersion=1]” key in the file header.

³ L. Liu et al. *ReaxFF-lg: Correction of the ReaxFF Reactive Force Field for London Dispersion, with Applications to the Equations of State for Energetic Materials*. J. Phys. Chem. A, 2011, 115 (40), pp 11016–11022. <https://doi.org/10.1021/jp201599t>

REAXFF ENGINE FEATURES VS. OLD STANDALONE PROGRAM

5.1 Introduction

Starting with AMS2018, ReaxFF is an engine for the AMS driver, thus sharing many of the features and input syntax with the other engines in the Amsterdam Modeling Suite.

Before AMS2018, ReaxFF was run as a standalone program. The older standalone program (“Old ReaxFF”) can still be run from the command-line, also in AMS2020. Some features are only available in this older program.

See also:

[Old Standalone ReaxFF manual](#)

The engine shares all core routines with the standalone program, guaranteeing identical energies and forces between these two codes.

5.2 Feature comparison

Some features of the old standalone ReaxFF program have been implemented into the AMS driver, others into the ReaxFF engine, and some are currently not available in the new implementation. The table below indicates how certain features can be activated.

| Feature | New implementation | Old implementation |
|--------------------------------|-----------------------------------|----------------------------|
| 0D, 1D, 2D periodicity | AMS driver | not available |
| ACKS2 | <i>force field file</i> (page 11) | old manual entry |
| Adsorption analysis | AMS driver | old manual entry |
| Bond boost | AMS driver | old manual entry |
| ChemTraYzer | AMS utilities | old manual entry |
| CMAES FF optimizer | ParAMS | old manual entry |
| CVHD | AMS driver | old manual entry |
| Elastic wall restraint | not available | old manual entry |
| eReaxFF | <i>force field file</i> (page 11) | old manual entry |
| External electric fields | AMS driver | old manual entry |
| Force-bias Monte Carlo | not available | old manual entry |
| Force field parametrization | ParAMS | old manual entry |
| Grand-canonical Monte Carlo | AMS driver | old manual entry |
| Local atomic temperature | not available | old manual entry |
| LG dispersion | <i>force field file</i> (page 12) | old manual entry |
| Molecular charge constraints | <i>ReaxFF Engine</i> (page 7) | old manual entry |
| Molecule gun | AMS driver | old manual entry |
| NEMD (thermal conductivity) | AMS driver | old manual entry |
| Per-atom stress tensor | not available | old manual entry |
| Tapered bond orders | <i>ReaxFF engine</i> (page 3) | old manual entry |
| Temperature profile along axis | AMS driver | old manual entry |
| Volume regimes | AMS driver | vregime.in Training Course |

5.3 Differences in execution

To run ReaxFF as an AMS engine (recommended), run the `ams` executable and specify `Engine ReaxFF`:

```
"$AMSBIN"/ams <<EOF
# ams input
Engine ReaxFF
  ForceField CHO.ff
EndEngine
EOF
```

To run ReaxFF as a standalone program (not recommended unless necessary), run the `reaxff` executable. The files `control`, `geo`, etc., must exist in the current working directory. For more information, see the [Old ReaxFF manual](#).

```
"$AMSBIN"/reaxff
```

PARALLELIZATION (MPI AND OPENMP)

ReaxFF, both as a program and as an AMS engine, has been parallelized using both MPI and OpenMP. MPI uses multiple processes to share the work, while OpenMP uses multiple threads within the same process. Each parallelization method has its pluses and minuses. The OpenMP usually has a lower overhead than MPI but MPI can be used on a distributed-memory machine (compute cluster). It is possible to combine both methods in a single job, which may lead to a lower performance because of the double overhead. For small systems pure OpenMP can be much faster than hybrid OpenMP+MPI or pure MPI because of the relatively high cost of MPI communication.

Number of OpenMP threads

The number of OpenMP threads is controlled by the `OMP_NUM_THREADS` environment variable. If `OMP_NUM_THREADS` is not defined the program will set the number of threads to the minimum of the default number of threads from the OpenMP library and the number of physical processor cores in the machine divided by the number of MPI processes running on it. The default number of threads returned by the OpenMP library depends on different factors: the number of the machine's virtual processors, the MPI and the OpenMP library used and the batch system, if any. For example, when running ReaxFF on a quad-core desktop computer with hyperthreading (8 virtual processors) with IntelMPI using 4 MPI processes, the default number returned by the Intel OpenMP library will usually be 2 because the library is aware of the fact that it is running under MPI. The same OpenMP library running under a different MPI run-time, for example OpenMPI, will probably set the default number of threads to 8. In both cases, ReaxFF will use one OpenMP thread per process because it counts only physical cores and is aware of the job's MPI configuration.

When running under a batch system the default number of OpenMP threads will depend on the quality of integration of the batch system with the MPI runtime and the OpenMP library. For example, when running an IntelMPI version under SLURM, the number of threads should be set using the `-cpus-per-task` option to set the number of threads.

The `OMP_NUM_THREADS` environment variable's value overrides any defaults or heuristics when present.

Recommendations

For single-node calculations we recommend using pure OpenMP. To this end, set the `NSCM` environment variable to 1 and set `OMP_NUM_THREADS` to the number of processors to use or leave it undefined to use all cores.

When running on multiple nodes we recommend using pure MPI. To this end, set the `OMP_NUM_THREADS` environment variable to 1 and set other MPI-related options as you would do for any other AMS job. This is especially important if you are using an MPI runtime environment loosely integrated with the cluster's batch system.

INCLUDED FORCE FIELDS

See also [Included force fields \(development version\)](#)

Description of ReaxFF force fields

Disclaimer: Using these forcefields for systems they have not been explicitly trained against may produce unrealistic results. Please see the full manuscripts for more detailed information.

The force field files used by the SCM version of ReaxFF are compatible with those used by the original ReaxFF code. So if you have the force field information from somewhere else you can just use it (save it in a text file, and select it in AMSinput via the Other... option).

There are currently two major groupings (i.e., the ReaxFF branches) of parameter sets that are intra-transferable with one another: (1) the combustion branch and (2) the aqueous (water) branch. The major difference between these two branches is in the O/H parameters, where the combustion branch focuses on accurately describing water as a gas-phase molecule, and the water branch is targeted at aqueous chemistry.

AB.ff: (H/O/N/B) Ammonia Borane M.R.Weismiller, A.C.T. van Duin, J. Lee, R.A. Yetter *ReaxFF Reactive Force Field Development and Applications for Molecular Dynamics Simulations of Ammonia Borane Dehydrogenation and Combustion* *J. Phys. Chem. A* 2010, 114, 5485-5492 (<http://dx.doi.org/10.1021/jp100136c>)

- QM data were generated describing the single and (if relevant) double and triple bond dissociation for all B/N/O/H combinations. These data were used to derive initial ReaxFF bond parameters, and all calculations were performed using DFT with the B3LYP functional and the Pople 6-311G** basis set.
- The training set was then extended with QM data describing angular distortions in a set of small AB-related (AB H3N-BH3) molecules. These data were used to derive the initial ReaxFF angular parameters.
- The training set was extended with reaction barriers for key reaction steps such as H2 release from AB, dimerization of H2B-NH2 and reaction energies associated with H2 release from AB and with AB oxidation.
- Branch: combustion.

AuCSOH.ff: (Au/C/S/O/H) J.A. Keith, D. Fantauzzi, T. Jacob, and A.C.T. van Duin *Reactive forcefield for simulating gold surfaces and nanoparticles* *Physical Review B* (2010) 81, 235404-1/235404-8 (<http://dx.doi.org/10.1103/PhysRevB.81.235404>)

- The original Au-Au parameters were extended by three publications:
- Au/O: K. Joshi, A.C.T. van Duin, and T. Jacob Development of a ReaxFF description of gold oxides and initial application to cold welding of partially oxidized gold surfaces *Journal of Materials Chemistry* 20, (2010), 10431-10437 <http://dx.doi.org/10.1039/C0JM01556C>
- Au/C/S/H: T.T. Jarvi, A.C.T. van Duin, K. Nordlund, and W.A. Goddard Development of interatomic ReaxFF potentials for Au-S-C-H systems *Journal of Physical Chemistry C* 115, (2011), 10315-10322 <http://dx.doi.org/10.1021/jp201496x>

- C/O/H/S: Rahaman, O., van Duin, A. C. T., Goddard, W. A., III, and Doren, D. J. Development of a ReaxFF reactive force field for glycine and application to solvent effect and tautomerization *Journal of Physical Chemistry B* 115 (2011), 249-261 <http://dx.doi.org/10.1021/jp108642r>
- The forcefield does not include Au/N parameters
- Branch: water.

CHO.ff: (C/H/O) Hydrocarbon oxidation K.Chenoweth, A.C.T. van Duin, W. A. Goddard *ReaxFF Reactive Force Field for Molecular Dynamics Simulations of Hydrocarbon Oxidation* *J. Phys. Chem. A* 2008, 112, 1040-1053 (<http://dx.doi.org/10.1021/jp709896w>)

- To obtain the H/C/O compound data required to extend the hydrocarbon-training set, DFT calculations were performed on the following systems: (a) dissociation energies for various bonds containing carbon, oxygen, and hydrogen. The ground state structure was obtained through full geometry optimization. Dissociation curves were calculated by constraining only the bond length of interest and re-optimization of the remaining internal coordinates. Optimization was also performed for the various angles and torsions associated with C/H/O interactions.
- Branch: combustion.

HCONSB.ff: (H/C/O/N/S/B) M.R. Weismiller, A.C.T. van Duin, J. Lee, and R.A. Yetter, *ReaxFF Reactive Force Field Development and Applications for Molecular Dynamics Simulations of Ammonia Borane Dehydrogenation and Combustion* *J. Phys. Chem. A* (2010), 114, 5485-5492. (<http://dx.doi.org/10.1021/jp100136c>)

- The parameters in this forcefield were extended/improved by two other publications:
- A.M. Kamat, A.C.T. van Duin, and A. Yakovlev *Molecular Dynamics Simulations of Laser-Induced Incandescence of Soot Using an Extended ReaxFF Reactive Force Field*. *Journal of Physical Chemistry A* (2010), 114, 12561-1257 <http://dx.doi.org/10.1021/jp1080302>
- F.Castro-Marcano, A.M. Kamat, M.F. Russo, A.C.T. van Duin, and J.P. Mathews *Combustion of an Illinois No. 6 Coal Char Simulated Using an Atomistic Char Representation and the ReaxFF Reactive Force Field*. *Combustion and Flame* (2012), 159, 23273-1285 <http://dx.doi.org/10.1016/j.combustflame.2011.10.022>
- The C/H/O parameters are the same as in the CHO forcefield, with added S/C, S/H and S/O descriptions. This force field was used in Castro et al, *Combustion and Flame* 2011
- The Boron and Nitrogen parameters are based on (but not identical to) the parameters used in Weismiller et al, *JPC-A* 2010.
- Branch: combustion.

CuCl-H2O.ff: (Cu/Cl/H/O) O.Rahaman, A.C.T. van Duin, V.S. Bryantsev, J.E. Mueller, S.D. Solares, W.A. Goddard III, and D.J. Doren *Development of a ReaxFF Reactive Force Field for Aqueous Chloride and Copper Chloride* *J. Phys. Chem. A* 114 (2010), 3556-3568 (<http://dx.doi.org/10.1021/jp9090415>)

- This forcefield is an extension of: A.C.T. van Duin, V.S. Bryantsev, M.S. Diallo, W.A. Goddard, O. Rahaman, D.J. Doren, D. Raymand, and K. Hermansson *Development and validation of a ReaxFF reactive force field for Cu cation/water interactions and copper metal/metal oxide/metal hydroxide condensed phases* *Journal of Physical Chemistry A* 2010, 114, 9507-9514 <http://dx.doi.org/10.1021/jp102272z>
- Branch: water.

FeOCHCl.ff: (Fe/O/C/H/Cl) M.Aryanpour, A.C.T. van Duin, J.D. Kubicki *Development of a Reactive Force Field for Iron-Oxyhydroxide Systems* *J. Phys. Chem. A* 2010, 114, 6298-6307 (<http://dx.doi.org/10.1021/jp101332k>)

- The Cl parameters were published by: O. Rahaman, A.C.T. van Duin, V.S. Bryantsev, J.E. Mueller, S.D. Solares, W.A. Goddard III, and D.J. Doren *Development of a ReaxFF Reactive Force Field for Aqueous Chloride and Copper Chloride* *J. Phys. Chem. A* 114 (2010), 3556-3568 <http://dx.doi.org/10.1021/jp9090415>

- The initial force field parameters for the Fe-Fe parameters were taken from an earlier force field development project on bulk-iron metal, based on DFT-calculations on antiferromagnetic BCC and FCC. The ReaxFF parameters have not been published yet, however the DFT data can be found in ref 31 of the above mentioned manuscript. The O/H parameters were taken from the ReaxFF bulk water description. The Fe/Fe and O/H parameters were kept fixed to these initial values, whereas the Fe/O parameters were reoptimized against the quantum mechanical results presented in the above mentioned manuscript.
- Detailed information on the force field parameters is given in the supporting information of the above mentioned manuscript.
- Branch: water.

HE.ff: (C/H/O/N) RDX/High Energy L.Z. Zhang, A.C.T. van Duin, S.V. Zybin, and W.A. Goddard *Thermal Decomposition of Hydrazines from Reactive Dynamics Using the ReaxFF Reactive Force Field* *Journal of Physical Chemistry B* (2009) 113, 10770-10778 (<http://dx.doi.org/10.1021/jp900194d>)

- Part of this forcefield is also published in: L.Z. Zhang, S.V. Zybin, A.C.T. van Duin, S. Dasgupta, W.A. Goddard, and E.M. Kober *Carbon Cluster Formation during Thermal Decomposition of Octahydro-1,3,5,7-tetranitro-1,3,5,7-tetrazocine and 1,3,5-Triamino-2,4,6-trinitrobenzene High Explosives from ReaxFF Reactive Molecular Dynamics Simulations* *Journal of Physical Chemistry A* (2009) 113, 10619-10640 <http://dx.doi.org/10.1021/jp901353a>
- The parameters of the nitramine ReaxFF are based on a large number of ab initio QM calculations. Over 40 reactions and over 1600 equilibrated molecules have been used; they are designed to characterize the atomic interactions under various environments likely and unlikely high energy each atom can encounter. The training set contains bond breaking and compression curves for all possible bonds, angle and torsion bending data for all possible cases, as well as crystal data.
- Please see the supplemental material from *Phys. Rev. Lett.* 2003, 91, 098301 for a detailed description of the parameterization of this force field.
- Branch: combustion.

HE2.ff: (C/H/O/N/S/Si) RDX/High Energy L.Z. Zhang, S.V. Zybin, A.C.T. van Duin, S. Dasgupta, W.A. Goddard, and E.M. Kober *Carbon Cluster Formation during Thermal Decomposition of Octahydro-1,3,5,7-tetranitro-1,3,5,7-tetrazocine and 1,3,5-Triamino-2,4,6-trinitrobenzene High Explosives from ReaxFF Reactive Molecular Dynamics Simulations* *Journal of Physical Chemistry A* (2009) 113, 10619-10640 (<http://dx.doi.org/10.1021/jp901353a>)

- Similar to HE.ff with additional parameters fitted for the TATB explosive
- Branch: combustion.

NaH.ff: (Na/H) J.G.O. Ojwang, R. Van Santen, G.J. Kramer, A.C.T. van Duin, and W.A. Goddard *Modeling the sorption dynamics of NaH using a reactive force field* *Journal of Chemical Physics* 2008, 128, 164714 (<http://dx.doi.org/10.1063/1.2908737>)

- This forcefield originally had a typo, defining the H-Na-Na angle twice. The same typo is in table 4 of the publication, but the text clearly mentions that the second line should define Na-H-Na instead.
- Branch: combustion.

NiCH.ff: (Ni/C/H) J.E. Mueller, A.C.T. van Duin, and W.A. Goddard III *Development and Validation of ReaxFF Reactive Force Field for Hydrocarbon Chemistry Catalyzed by Nickel* *J. Phys. Chem. C* 2010, 114, 4939-4949 (<http://dx.doi.org/10.1021/jp9035056>)

- Branch: combustion.

SiOH.ff: (Si/O/H) J.C. Fogarty, H.M. Aktulga, A.Y. Grama, A.C.T. van Duin, S.A. Pandit *A reactive molecular dynamics simulation of the silica-water interface* *J. Chem. Phys.* 2010, 132, 174704 (<http://dx.doi.org/10.1063/1.3407433>)

- This force field was trained to model the interaction of water at the SiO₂ surface, with specific emphasis on proton-transfer reactions. Updated parameters were fitted for all Si/O/H bond, angle, and torsion interactions as well, in addition to the dissociation of a water molecule from a single Si(OH)₄ molecule and reaction energies for the polymerization of Si(OH)₄
- Branch: water.

SiC.ff: (Si/C/O/H/N/S) D.Newsome, D. Sengupta, H. Foroutan, M.F. Russo, and A.C.T. van Duin *Oxidation of Silicon Carbide by O₂ and H₂O: A ReaxFF Reactive Molecular Dynamics Study, Part I* *Journal of Physical Chemistry* 2012 116, 16111-16121 (<http://dx.doi.org/10.1021/jp306391p>)

- The included forcefield is based on the Newsome reference, with slightly improved parameters by van Duin et al.
- Branch: combustion.

VOCH.ff: (V/O/C/H) K.Chenoweth, A.C.T. van Duin, P. Persson, M.J. Cheng, J. Oxgaard, W.A. Goddard *Development and Application of a ReaxFF Reactive Force Field for Oxidative Dehydrogenation on Vanadium Oxide Catalysts* *J. Phys. Chem. C*, 2008, 112, 14645-14654 (<http://dx.doi.org/10.1021/jp802134x>)

- The ReaxFF force field parameters have been fit to a large quantum mechanics (QM) training set containing over 700 structures and energetics related to bond dissociations, angle and dihedral distortions, and reactions between hydrocarbons and vanadium oxide clusters. In addition, the training set contains charge distributions for small vanadium oxide clusters and the stabilities of condensed-phase systems including V₂O₅, VO₂, and V₂O₃ in addition to metallic V (V₀).
- Branch: combustion.

ZnOH.ff: (Zn/O/H) D.Raymand, A.C.T. van Duin, M. Baudin, K. Hermansson *A reactive force field (ReaxFF) for zinc oxide* *Surface Science* 2008, 602, 1020-1031 (<http://dx.doi.org/10.1016/j.susc.2007.12.023>)

- updated version published by: D. Raymand, A.C.T. van Duin, D. Spangberg, W.A. Goddard, K. Hermansson *Water adsorption on stepped ZnO surfaces from MD simulation* *Surface Science* 2010, 604, 9-10, 741-752 <http://dx.doi.org/10.1016/j.susc.2009.12.012>
- Based on QM calculations for Zn(s), ZnO(s), and Zn hydroxide clusters [Zn(OH)₂ and O(ZnOH)₂], ReaxFF parameters were generated for Zn-O and Zn-Zn bond energies and for Zn-O-Zn, O-Zn-O, O-Zn-Zn and Zn-O-H valence angle energies.
- QM calculations were performed for the four crystal polymorphs of the wurtzite, zincblende, rocksalt and caesium chloride structures (the structures are also referred to as h-ZnS, c-ZnS, NaCl and CsCl, respectively).
- Branch: water.

Al-H₂O.ff: (Al/H/O) M.Russo, R. Li, M. Mench, and A.C.T. van Duin *Molecular Dynamic Simulation of Aluminum-Water Reactions Using the ReaxFF Reactive Force Field* *International Journal of Hydrogen Energy* 36 (2011), 5828-5835 (<http://dx.doi.org/10.1016/j.ijhydene.2011.02.035>)

- Branch: water.

CaSiAlO.ff: (C/H/O/Fe/Cl/Si/Al/Ca) M.C. Pitman and A.C.T. van Duin *Dynamics of Confined Reactive Water in Smectite Clay-Zeolite Composites* *J. Am. Chem. Soc.*, 2012, 134 (6), 3042-3053 (<http://dx.doi.org/10.1021/ja208894m>)

- Branch: water.

dispersion/CHONSSi-Ig.ff: (C/H/O/N/S/Si) L.Liu, Y. Liu, S.V. Zybin, H. Sun, and W.A. Goddard III *ReaxFF-Ig: Correction of the ReaxFF Reactive Force Field for London Dispersion, with Applications to the Equations of State for Energetic Materials* *The Journal of Physical Chemistry A*, 2011, 115(40), 11016-11022 (<http://dx.doi.org/10.1021/jp201599t>)

- This forcefield adds London dispersion correction terms to reaxFF, and is optimized for the energetic materials RDX, PETN, TATB, and NM plus graphite, polyethylene, solid carbon dioxide, and solid N₂, using the low temperature crystal structures to determine the lg correction parameters.
- Branch: combustion.

CHOFeAlNiCuS.ff: (C/H/O/Fe/Al/Ni/Cu/S) O.Rahaman, A.C.T. van Duin, W.A. Goddard III, and D.J. Doren *Development of a ReaxFF reactive force field for glycine and application to solvent effect and tautomerization* *Journal of Physical Chemistry B* 115 (2011), 249-261. (<http://dx.doi.org/10.1021/jp204894m>)

- C/O/H parameters only. The Cu/Fe/Al/Ni parameters are from: Y.K. Shin, H. Kwak, C. Zou, A.V. Vasenkov, and A.C.T. van Duin *Development and Validation of a ReaxFF Reactive Force Field for Fe/Al/Ni Alloys: Molecular Dynamics Study of Elastic Constants, Diffusion, and Segregation* *J. Phys. Chem. A*, 2012, 116 (49), pp 12163–12174 <http://dx.doi.org/10.1021/jp308507x>
- Not all cross-terms between the two forcefield files are defined, which might cause problems if the system has (for example) C-Cu interactions.
- Branch: water.

AuSCH_2011.ff: (Au/S/C/H) T.T. Jarvi, A.C.T. van Duin, K. Nordlund, and W.A. Goddard III, *Development of Interatomic ReaxFF Potentials for Au-S-C-H Systems* *J. Phys. Chem. A*, 115, 10315-10322 (2011) (<http://dx.doi.org/10.1021/jp201496x>)

- Branch: combustion.

AuSCH_2013.ff: (Au/S/C/H) Gyun-Tack Bae and Christine M. Aikens *Improved ReaxFF Force Field Parameters for Au-S-C-H Systems* *Journal of Physical Chemistry A* 2013 117 (40), 10438-10446 (<http://dx.doi.org/10.1021/jp405992m>)

- Based upon: T.T. Jarvi, A.C.T. van Duin, K. Nordlund, and W.A. Goddard *Development of interatomic ReaxFF potentials for Au-S-C-H systems*. *Journal of Physical Chemistry C* 115, (2011), 10315-10322.
- yields improvements for bond bending potential energy surfaces
- aims to agree with DFT geometries of small clusters and gold-thiolate nanoparticles
- Branch: combustion.

PDMSDecomp.ff: (C/H/O/Si) K.Chenoweth, S. Cheung, A.C.T. van Duin, W.A. Goddard III, and E.M. Kober *Simulations on the Thermal Decomposition of a Poly(dimethylsiloxane) Polymer Using the ReaxFF Reactive Force Field* *J. Am. Chem. Soc.*, 2005, 127 (19), pp 7192-7202 (<http://dx.doi.org/10.1021/ja050980t>)

- Specialized forcefield, designed to “investigate the failure of the poly(dimethylsiloxane) polymer (PDMS) at high temperatures and pressures and in the presence of various additives”
- Line from the torsion block was referring to non-existent atoms from the atomic block and thus was removed.
- Branch: combustion.

TiOCHNCl.ff: (C/H/O/N/S/Mg/P/Na/Ti/Cl/F) S.Y. Kim, A.C.T. van Duin, and J.D. Kubicki *Molecular dynamics simulations of the interactions between TiO₂ nanoparticles and water with Na⁺ and Cl⁻, methanol, and formic acid using a reactive force field* *Journal of Materials Research / Volume 28 / Issue 03 / 2013*, pp 513-520 (<http://dx.doi.org/10.1557/jmr.2012.367>)

- used for simulating TiO₂(both rutile and anatase) nanoparticles with water, methanol, and formic acid
- The force field was validated by comparing water dissociative adsorption percentage and bond length between Na-O with density functional theory (DFT) and experimental results
- Branch: water.

PtCH.ff: (C/H/Pt) C.F. Sanz-Navarro, P. Astrand, De Chen, M. Ronning, A.C.T. van Duin, T. Jacob, and W.A. Goddard III *Molecular Dynamics Simulations of the Interactions between Platinum Clusters and Carbon Platelets* J. Phys. Chem. A 112, 1392-1402 (2008) (<http://dx.doi.org/10.1021/jp074806y>)

- Branch: combustion.

BaYZrCHO.ff: (C/H/O/Ba/Zr/Y) A.C.T. van Duin, B.V. Merinov, S.S. Jang, and W.A. Goddard III *ReaxFF Reactive Force Field for Solid Oxide Fuel Cell Systems with Application to Oxygen Ion Transport in Yttria-Stabilized Zirconia* J. Phys. Chem. A, 112, 3133-3140 (2008) (<http://dx.doi.org/10.1021/jp076775c>)

- Branch: combustion.

CHONSSiPtZrNiCuCo.ff: (C/H/O/N/S/Si/Pt/Zr/Ni/Cu/Co) K.D. Nielson, A.C.T. van Duin, J. Oxgaard, W.Q. Deng, and W.A. Goddard III *Development of the ReaxFF Reactive Force Field for Describing Transition Metal Catalyzed Reactions, with Application to the Initial Stages of the Catalytic Formation of Carbon Nanotubes* J. Phys. Chem. A, 109, 493-499 (2005) (<http://dx.doi.org/10.1021/jp046244d>)

- Branch: combustion.

Glycine.ff: (C/H/O/N) O.Rahaman, A.C.T. van Duin, W.A. Goddard III, and D.J. Doren, *Development of a ReaxFF Reactive Force Field for Glycine and Application to Solvent Effect and Tautomerization* J. Phys. Chem. B, 115, 249-261 (2011) (<http://dx.doi.org/10.1021/jp108642r>)

- Line from the valence angle block was referring to non-existent atoms from the atomic block and thus was removed.
- Branch: water.

SiONH.ff: (C/H/O/N/Si/S) A.D. Kulkarni, D.G. Truhlar, S.G. Srinivasan, A.C.T. van Duin, P. Norman, and T.E. Schwartzentruber *Oxygen Interactions with Silica Surfaces: Coupled Cluster and Density Functional Investigation and the Development of a New ReaxFF Potential* J. Phys. Chem. C, 2013, 117 (1), pp 258-269 (<http://dx.doi.org/10.1021/jp3086649>)

- Aimed at oxygen interactions with realistic silica surfaces
- Lines from the valence angle block was referring to non-existent atoms from the atomic block and thus was removed.
- Branch: combustion.

CHOFe.ff: (C/H/O/Fe/Cl/Si/Al) Chenyu Zou, A.C.T. Van Duin *Investigation of Complex Iron Surface Catalytic Chemistry Using the ReaxFF Reactive Force Field Method* JOM, December 2012, Volume 64, Issue 12, pp 1426-1437 (<http://dx.doi.org/10.1007/s11837-012-0463-5>)

- only the parameters for Fe (and crossterms) differ from the CHOAlSi.ff forcefield
- Branch: water.

CHOAlSi.ff: (C/H/O/Fe/Cl/Si/Al) F.Castro-Marcanao, A.C.T. van Duin *Comparison of thermal and catalytic cracking of 1-heptene from ReaxFF reactive molecular dynamics simulations* Combustion and Flame, Volume 160, Issue 4, April 2013, Pages 766-775 (<http://dx.doi.org/10.1016/j.combustflame.2012.12.007>)

- only the parameters for Fe (and crossterms) differ from the CHOFe.ff forcefield
- Branch: water.

CHOLi.ff: (C/H/O/N/S/Mg/P/Na/Li) D.Bedrov, G.D. Smith, A.C.T. van Duin *Reactions of Singly-Reduced Ethylene Carbonate in Lithium Battery Electrolytes: A Molecular Dynamics Simulation Study Using the ReaxFF* Journal of Physical Chemistry A, 2012, 116 (11), pp 2978-2985 (<http://dx.doi.org/10.1021/jp210345b>)

- specifically generated for simulating Lithium battery electrolytes
- must be used in combination with the MOLCHARGE keyword to set a charge restraint on Li and CO3!
- Branch: water.

SiOAlLi.ff: (H/O/Si/Al/Li) B.Narayanan, A.C.T. van Duin, B.B. Kappes, I.E. Reimanis and C.V. Ciobanu *A reactive force field for lithium-aluminum silicates with applications to eucryptite phases* *Modelling and Simulation in Materials Science and Engineering* 2012 20 015002 (<http://dx.doi.org/10.1088/0965-0393/20/1/015002>)

- Branch: water.

PdO.ff: (Pd/O) T.P. Senftle, R.J. Meyer, M.J. Janik and A.C.T. van Duin *Development of a ReaxFF potential for Pd/O and application to palladium oxide formation* *The Journal of Chemical Physics* 139, 044109 (2013) (<http://dx.doi.org/10.1063/1.4815820>)

- used for studying Oxidation states of Pd nanoparticles, surfaces and bulk configurations with a GCMC method
- Branch: combustion.

PdH.ff: (Pd/H) T.P. Senftle, M.J. Janik and A.C.T. van Duin *A ReaxFF Investigation of Hydride Formation in Palladium Nanoclusters via Monte Carlo and Molecular Dynamics Simulations* *The Journal of Physical Chemistry C*, 2014, 118 (9), pp 4967-4981 (<http://dx.doi.org/10.1021/jp411015a>)

- used in combination with a GCMC method
- Branch: combustion.

Co.ff: (Co) Xue-Qing Zhang, E. Iype, S.V. Nedeia, A.P.J. Jansen, B.M. Szyja, E.J.M. Hensen, and R.A. van Santen *Site Stability on Cobalt Nanoparticles: A Molecular Dynamics ReaxFF Reactive Force Field Study* *The Journal of Physical Chemistry C*, 2014, 118 (13), pp 6882-6886 (<http://dx.doi.org/10.1021/jp500053u>)

- forcefield was generated using a recently developed Monte Carlo algorithm with simulated annealing.
- Branch: combustion.

CHONSMgPNaCuCl.ff: (C/H/O/N/S/Mg/P/Na/Cu/Cl) Susanna Monti, Cui Li, and Vincenzo Carravetta *Reactive Dynamics Simulation of Monolayer and Multilayer Adsorption of Glycine on Cu(110)* *J. Phys. Chem. C*, 2013, 117 (10), pp 5221-5228 (<http://dx.doi.org/10.1021/jp312828d>)

- Reactive MD-force field for amino acids on copper
- Branch: water.

CHOSMoNiLiBFPN.ff: (C/H/O/S/Mo/Ni/Li/B/F/P/N) Md M. Islam, V.S. Bryantsev, A.C.T. van Duin *ReaxFF Reactive Force Field Simulations on the Influence of Teflon on Electrolyte Decomposition during Li/SWCNT Anode Discharge in Lithium-Sulfur Batteries* *J. Electrochem. Soc.* 2014 volume 161, issue 8, E3009-E3014 (<http://dx.doi.org/10.1149/2.005408jes>)

- forcefield for Electrochemistry in Li-S batteries
- Branch: combustion.

CHONSSiNaFZr.ff: (C/H/O/N/S/Si/Na/F/Zr) A.Rahnamoun and A.C.T. van Duin *Reactive Molecular Dynamics Simulation on the Disintegration of Kapton, POSS Polyimide, Amorphous Silica, and Teflon during Atomic Oxygen Impact Using the Reaxff Reactive Force-Field Method* *J. Phys. Chem. A*, 2014, 118 (15), pp 2780-2787 (<http://dx.doi.org/10.1021/jp4121029>)

- comments in the forcefield file: interactions with water and Na+ Fogarty et al. JCP-2010 ; with glycine + C/H/F parameters; Si-F bond/offdiag/angle parameters; Si-S dummy parameters + S-O-H parameters(Yun 2012 Oct8) + H-F bond/offdiag (Jan14 2013 Joon) Jan31: added Zr/O/H/C
- Branch: water.

TiClOH.ff: (C/H/O/N/S/Mg/P/Na/Ti/Cl/F) Sung-Yup Kim and A.C.T. van Duin *Simulation of Titanium Metal/Titanium Dioxide Etching with Chlorine and Hydrogen Chloride Gases Using the ReaxFF Reactive Force Field* *J. Phys. Chem. A*, 2013, 117 (27), pp 5655-5663 (<http://dx.doi.org/10.1021/jp4031943>)

- adaptation/evolution of the TiOCHNCl.ff forcefield by Kim, S.-Y. et al.

- Branch: water.

CHONSSiNaAl.ff: (C/H/O/N/S/Si/Na/Al) C.Bai, L. Liu, and H. Sun *Molecular Dynamics Simulations of Methanol to Olefin Reactions in HZSM-5 Zeolite Using a ReaxFF Force Field* *J. Phys. Chem. C*, 2012, 116 (12), pp 7029-7039 (<http://dx.doi.org/10.1021/jp300221j>)

- used to simulate methanol to olefin (MTO) reactions in H-ZSM-5 zeolite
- Branch: water.

undocumented/NiCH.ff: (Ni/C/H/O/N/S/F/Pt/Cl) Unknown *No Name* Not published (<http://>)

- This forcefield is from april 2009, and is not published
- Branch: combustion.

LiS.ff: (Li/S) Md M. Islam, A. Ostadhossein, O. Borodin, A.T. Yeates, W.W. Tipton, R.G. Hennig, N. Kumar, and A.C.T. van Duin *ReaxFF molecular dynamics simulations on lithiated sulfur cathode materials* *Phys. Chem. Chem. Phys.*, 2015, 17, 3383-3393 (<http://dx.doi.org/10.1039/C4CP04532G>)

- Developed for and used to study Sulfur cathode behaviour in Li battery cells
- Branch: combustion.

CHONSSiPtNiCuCoZrYBa.ff: (C/H/O/N/S/Si/Pt/Ni/Cu/Co/Zr/Y/Ba) B.V. Merinov, J.E. Mueller, A.C.T. van Duin, Qi An, and W.A. Goddard III *ReaxFF Reactive Force-Field Modeling of the Triple-Phase Boundary in a Solid Oxide Fuel Cell* *J. Phys. Chem. Lett.*, 2014, 5 (22), pp 4039-4043 (<http://dx.doi.org/10.1021/jz501891y>)

- Force field was developed by combining the YSZ and Ni/C/H descriptions
- From the summary: “The products obtained in our simulations are the same as those in experiment, which indicates that the developed ReaxFF potential properly describes complex physicochemical processes, such as the oxide-ion diffusion, fuel conversion, water formation reaction, coking, and delamination, occurring at the TPB and can be recommended for further computational studies of the fuel/electrode/electrolyte interfaces in a SOFC”
- The Aa atom type is a rename of the Zr atom type, which was defined twice.
- Branch: combustion.

CHONSSiNaP.ff: (C/H/O/N/S/Si/Na/P) Bo Zhang, A.C.T. van Duin and J.K. Johnson *Development of a ReaxFF Reactive Force Field for Tetrabutylphosphonium Glycinate/CO₂ Mixtures* *J. Phys. Chem. B*, 2014, 118 (41), pp 12008-12016 (<http://dx.doi.org/10.1021/jp5054277>)

- The forcefield file mentions “Gly with dummy N-P parameters”
- It was developed for studying Carbon dioxide interactions with the ionic liquid tetrabutylphosphonium glycinate, both physical and chemical absorption.
- Several lines from valence angle block were referring to non-existent atoms from the atomic block and thus were removed.
- Branch: combustion.

CHOLi_2.ff: (C/H/O/Li) M.Raju, P. Ganesh, P.R.C. Kent, and A.C.T. van Duin *Reactive Force Field Study of Li/C Systems for Electrical Energy Storage* *J. Chem. Theory Comput.*, 2015, 11 (5), pp 2156-2166 (<http://dx.doi.org/10.1021/ct501027v>)

- Used for studying Li/C systems with GCMC and MD
- Also contains parameters for “Vi” and “GI”, but these virtual elements are not mentioned in the paper
- Parameters were fitted using a training set consisting, amongst others, of Li binding energies on pristine graphene and graphite, Li migration pathways in graphite and Li dissociation pathways in different hydrocarbons

- The forcefield was validated by a side-by-side comparison of ReaxFF and DFT energies for Li binding on a divacancy, and ReaxFF and DFT ground-state configurations for stage II and stage I stacking in graphite obtained using GCMC simulations
- The forcefield reproduces the in-plane Li ordering as well as the graphite stacking sequence for stage II and stage I compounds
- Branch: water.

CHONSiCaCsKSrNaMgAlCu.ff: (C/H/O/N/S/Si/Ca/Cs/K/Sr/Na/Mg/Al/Cu) G.M. Psfogiannakis, J.F. McCleerey, E. Jaramillo and A.C.T. van Duin *ReaxFF Reactive Molecular Dynamics Simulation of the Hydration of Cu-SSZ-13 Zeolite and the Formation of Cu Dimers* *J. Phys. Chem. C*, 2015, 119 (12), pp 6678-6686 (<http://dx.doi.org/10.1021/acs.jpcc.5b00699>)

- This Cu/Si/Al/O/H forcefield was developed for and used in MD simulations of the hydration of Cu-exchanged SSZ-13 catalyst.
- The force field was developed by merging and expanding previously tested and published ReaxFF force fields for Si/Al/O/H systems and Cu/O/H systems (citations 19-26 of the publication)
- This forcefield is an extension of K.L. Joshi et al 2014, <http://dx.doi.org/10.1039/C4CP02612H>, all non-Cu parameters are the same.
- Branch: water.

HOSMg.ff: (H/O/S/Mg) E.Iype, M. Hütter, A.P.J. Jansen, S.V. Nedea and C.C.M. Rindt *Parameterization of a reactive force field using a Monte Carlo algorithm* *J. Comput. Chem.*, 2013, 34: 1143-1154 (<http://dx.doi.org/10.1002/jcc.23246>)

- This forcefield is optimized with a metropolis Monte-Carlo algorithm with simulated annealing to search for the optimum parameters for the ReaxFF force field in a high- dimensional parameter space.
- The optimization is done against a set of quantum chemical data for MgSO₄ hydrates.
- Branch: combustion.

CHONSMgPNaCuCl_v2.ff: (C/H/O/N/S/Mg/P/Na/Cu/Cl) S.Monti, A. Corozzi, P. Fristrup, K.L. Joshi, Yun Kyung Shin, P. Oelschlaeger, A.C.T. van Duin and V. Baronee *Exploring the conformational and reactive dynamics of biomolecules in solution using an extended version of the glycine reactive force field* *Phys. Chem. Chem. Phys.*, 2013,15, 15062-15077 (<http://dx.doi.org/10.1039/C3CP51931G>)

- This forcefield is an extension of CHONSMgPNaCuCl.ff by S. Monti et al., *J. Phys. Chem. C*, 2013, 117 (10), pp 5221-5228, <http://dx.doi.org/10.1021/jp312828d>
- Developed for peptide and protein simulations
- Branch: water.

OPt.ff: (O/Pt) D.Fantauzzi, J. Bandlow, L. Sabo, J.E. Mueller, A.C.T. van Duin and T. Jacob *Development of a ReaxFF potential for Pt-O systems describing the energetics and dynamics of Pt-oxide formation* *Phys. Chem. Chem. Phys.*, 2014,16, 23118-23133 (<http://dx.doi.org/10.1039/C4CP03111C>)

- Pt-Pt parameters for bulk platinum phases, low & high-index platinum surfaces and nanoclusters.
- O-Pt parameters for bulk platinum oxides, as well as oxygen adsorption and oxide formation on Pt(111) terraces and the {111} and {100} steps connecting them.
- Branch: combustion.

CHONSMgPNaTiClF.ff: (C/H/O/N/S/Mg/P/Na/Ti/Cl/F) Stijn Huygh, Annemie Bogaerts, Adri C.T. van Duin and Erik C. Neyts *Development of a ReaxFF reactive force field for intrinsic point defects in titanium dioxide* *Computational Materials Science*, Volume 95, December 2014, Pages 579-591, ISSN 0927-0256 (<http://dx.doi.org/10.1016/j.commatsci.2014.07.056>)

- Forcefield developed for studying the influence of intrinsic point defects on the chemistry with TiO₂ condensed phases.
- Forcefield seems to be based on TiOCHNCl.ff, <http://dx.doi.org/10.1557/jmr.2012.367>
- Branch: water.

LiSi.ff: (Li/Si) A.Ostadossein, E.D. Cubuk, G.A. Tritsarlis, E. Kaxiras, S. Zhanga and A.C.T. van Duin *Stress effects on the initial lithiation of crystalline silicon nanowires: reactive molecular dynamics simulations using ReaxFF* Phys. Chem. Chem. Phys., 2015, 17, 3832-3840 (<http://dx.doi.org/10.1039/C4CP05198J>)

- Branch: combustion.

CHOFeAlNiCuSCr.ff: (C/H/O/Fe/Al/Ni/Cu/S/Cr) Y.K. Shin, H. Kwak, A.V. Vasenkov, D. Sengupta and A.C.T. van Duin *Development of a ReaxFF Reactive Force Field for Fe/Cr/O/S and Application to Oxidation of Butane over a Pyrite-Covered Cr₂O₃ Catalyst* ACS Catalysis, 2015, 5 (12), pp 7226-7236 (<http://dx.doi.org/10.1021/acscatal.5b01766>)

- Forcefield optimized for Fe/Cr/O/S
- Branch: water.

CHOFeAlNiCuSCr_v2.ff: (C/H/O/Fe/Al/Ni/Cu/S/Cr) Ni-O-vacancy C.Zou et al. *Molecular dynamics simulations of the effects of vacancies on nickel self-diffusion, oxygen diffusion and oxidation initiation in nickel, using the ReaxFF reactive force field* Acta Materialia, Volume 83, 15 January 2015, Pages 102-112 (<http://dx.doi.org/10.1016/j.actamat.2014.09.047>)

- Forcefield optimized for Ni/O, trained with a QM data on Ni, NiO and vacancies
- The non-carbon parameters are the same as in CHOFeAlNiCuSCr_v3.ff
- Branch: water.

CHOFeAlNiCuSCr_v3.ff: (C/H/O/Fe/Al/Ni/Cu/S/Cr) F.Tavazza, T.P. Senftle, C. Zou, C.A. Becker and A.C.T. van Duin *Molecular Dynamics Investigation of the Effects of Tip-Substrate Interactions during Nanoindentation* J. Phys. Chem. C, 2015, 119 (24), pp 13580-13589 (<http://dx.doi.org/10.1021/acs.jpcc.5b01275>)

- Combination of the C.ff (condensed carbon) forcefield with Ni/C/O/H parameters
- The non-carbon parameters are the same as in CHOFeAlNiCuSCr_v2.ff
- Branch: water.

C.ff: (C) C-2013 S.G. Srinivasan, A.C.T. van Duin and P. Ganesh *Development of a ReaxFF Potential for Carbon Condensed Phases and Its Application to the Thermal Fragmentation of a Large Fullerene* J. Phys. Chem. A, 2015, 119 (4), pp 571-580 (<http://dx.doi.org/10.1021/jp510274e>)

- Forcefield designed for modeling Carbon condensed phases
- Branch: combustion.

CHONSSiGe.ff: (C/H/O/N/S/Si/Ge) G.Psofogiannakis and A.C.T. van Duin *Development of a ReaxFF reactive force field for Si/Ge/H systems and application to atomic hydrogen bombardment of Si, Ge, and SiGe (100) surfaces* Surface Science 2016, Vol. 646, pp 253-260 (<http://dx.doi.org/10.1016/j.susc.2015.08.019>)

- Forcefield designed for bombardment of Si, Ge and SiGe surfaces with atomic hydrogen.
- Branch: combustion.

CHONSFPtCINi.ff: (C/H/O/N/S/F/Pt/Cl/Ni) Water-Pt-Ni-Nafion D.Fantauzzi, J.E. Mueller, L. Sabo, A.C.T. van Duin and T. Jacob *Surface Buckling and Subsurface Oxygen: Atomistic Insights into the Surface Oxidation of Pt(111)* ChemPhysChem, 2015, Vol.16: 2797-2802 (<http://dx.doi.org/10.1002/cphc.201500527>)

- extension of the OPt.ff forcefield parameters
- Branch: water.

CHONSSiPtZrNiCuCoHeNeArKrXe.ff: (C/H/O/N/S/Si/Pt/Zr/Ni/Cu/Co/He/Ne/Ar/Kr/Xe) A.M. Kamat, A.C.T. van Duin and A. Yakovlev *Molecular Dynamics Simulations of Laser-Induced Incandescence of Soot Using an Extended ReaxFF Reactive Force Field* *J. Phys. Chem. A*, 2010, 114 (48), pp 12561-12572 (<http://dx.doi.org/10.1021/jp1080302>)

- forcefield designed for the study of Laser-induced incandescence of soot
- Branch: combustion.

CHOSFCIN.ff: (C/H/O/S/F/Cl/N) M.A. Wood, A.C.T. van Duin and A. Strachan *Coupled Thermal and Electromagnetic Induced Decomposition in the Molecular Explosive alpha-HMX; A Reactive Molecular Dynamics Study* *J. Phys. Chem. A*, 2014, 118 (5), pp 885-895 (<http://dx.doi.org/10.1021/jp406248m>)

- forcefield designed for studying the combustion of the high-energy material a-HMX
- Branch: combustion.

Mue2016.ff: (C/H/O/S) Julian Mueller and Bernd Hartke *ReaxFF Reactive Force Field for Disulfide Mechanochemistry, Fitted to Multireference ab Initio Data;* *J. Chem. Theory Comput.*, 2016, xxx, xxx (<http://dx.doi.org/10.1021/acs.jctc.6b00461>)

- forcefield for studying S-S bond ruptures in mechanophores upon mechanical stress. Ambient conditions, both in gas phase and toluene solvent.
- Branch: combustion.

CBN.ff: (C/H/B/N) Sung Jin Pai, Byung Chul Yea and Sang Soo Han *Reactive force field for the improved design of liquid CBN hydrogen storage materials* *Phys. Chem. Chem. Phys.*, 2016, 18, pp 1818-1827 (<http://dx.doi.org/10.1039/C5CP05486A>)

- forcefield for studying liquid CBN (carbon-boron-nitrogen) hydrogen-storage materials.
- Branch: combustion.

AgZnO.ff: (C/H/O/N/Si/Cu/Ag/Zn) A.Lloyd, D. Cornil, A.C.T. van Duin, D. van Duin, R. Smith, S.D. Kenny, J. Cornil and D. Beljonne *Development of a ReaxFF potential for Ag/Zn/O and application to Ag deposition on ZnO* *Surface Science*, 2016, 645, pp 67-73 (<http://dx.doi.org/10.1016/j.susc.2015.11.009>)

- ReaxFF potential for Ag/Zn/O used to study Ag deposition on ZnO.
- Branch: water.

AlCHO.ff: (Al/C/H/O) Sungwook Hong and Adri C. T. van Duin *Atomistic-Scale Analysis of Carbon Coating and Its Effect on the Oxidation of Aluminum Nanoparticles by ReaxFF-Molecular Dynamics Simulations* *J. Phys. Chem. C*, 2016, 120 (17), pp 9464-9474 (<http://dx.doi.org/10.1021/acs.jpcc.6b00786>)

- ReaxFF potential for Al/C interactions. Used to investigate carbon coating and its effect on the oxidation of aluminum nanoparticles (ANPs)
- Branch: water.

CHNa.ff: (C/H/Na) E.Hjertenaes, A.Q. Nguyen and H. Koch *A ReaxFF force field for sodium intrusion in graphitic cathodes* *Phys. Chem. Chem. Phys.*, 2016, 18, pp 31431-31440 (<http://dx.doi.org/10.1039/C6CP06774C>)

- The force field is applied in hybrid grand canonical Monte Carlo-molecular dynamics (GC-MC/MD) simulations of model systems representative of sodium intrusion in graphitic carbon cathodes used in aluminium electrolysis.
- Branch: combustion.

CuBTC.ff: (C/H/O/N/S/Mg/P/Na/Cu) L.Huang, T. Badosz, K. L. Joshi, A. C. T. van Duin and K. E. Gubbins *Reactive adsorption of ammonia and ammonia/water on CuBTC metal-organic framework: A ReaxFF molecular dynamics simulation* *J. Chem. Phys.*, 2013, 138, 034102 (<http://dx.doi.org/10.1063/1.4774332>)

- The force field was used to study reactive adsorption of NH₃ on the dehydrated CuBTC metal-organic framework.
- Branch: water.

CHONSMgPNaTiClFAu.ff: (C/H/O/N/S/Mg/P/Na/Ti/Cl/F/Au) Susanna Monti, Vincenzo Carravetta, and Hans Ågren *Simulation of Gold Functionalization with Cysteine by Reactive Molecular Dynamics* *J. Phys. Chem. Lett.*, 2016, 7 (2), pp 272-276 (<http://dx.doi.org/10.1021/acs.jpcclett.5b02769>)

- The force field was designed to study gold-protein interactions in water.

HOSiAILi.ff: (H/O/Si/Al/Li) Alireza Ostadhossein, Sung-Yup Kim, Ekin D. Cubuk, Yue Qi, and Adri C. T. van Duin *Atomic Insight into the Lithium Storage and Diffusion Mechanism of SiO₂/Al₂O₃ Electrodes of Lithium Ion Batteries: ReaxFF Reactive Force Field Modeling* *J. Phys. Chem. A*, 2016, 120 (13), pp 2114-2127 (<http://dx.doi.org/10.1021/acs.jpca.5b11908>)

- Developed for studying the energetics and kinetics of lithiation, as well as Li transportation within the crystalline/amorphous silica and alumina phases.

CHArHeNeKr.ff: (C/H/Ar/He/Ne/Kr) Kichul Yoon, A. Rahnamoun, J.L. Swett, V. Iberi, D.A. Cullen, I.V. Vlas-siouk, A. Belianinov, S. Jesse, X. Sang, O.S. Ovchinnikova, A.J. Rondinone, R.R. Unocic, and A.C.T. van Duin *Atomistic-Scale Simulations of Defect Formation in Graphene under Noble Gas Ion Irradiation* *ACS Nano*, 2016, 10 (9), pp 8376-8384 (<http://dx.doi.org/10.1021/acs.nano.6b03036>)

- Developed for studying noble gas ion irradiation of graphene and the subsequent effects of annealing. Lattice defects including nanopores were generated.

CHO-radiation.ff: (C/H/O) Roger Smith, K. Jolley, C. Latham, M. Heggie, A van Duin, D. van Duin, Houzheng Wu *A ReaxFF carbon potential for radiation damage studies* *Nuclear Instruments and Methods in Physics Research Section B: Beam Interactions with Materials and Atoms*, Volume 393, 15 February 2017, Pages 49-53, (<http://dx.doi.org/10.1016/j.nimb.2016.11.007>)

- Developed forcefield reproduces the formation energies of many of the defects predicted by the ab initio calculations of energetic impacts and collision cascades in graphite.
- Forcefield reproduces the formation energies of many of the defects predicted by the ab initio calculations and the energy pathways between different defect states, which are important for investigating long term defect evolution.

HOTiPd.ff: (H/O/Ti/Pd) Rafik Addou, T.P. Senftle, N. O'Connor, M.J. Janik, A.C.T. van Duin, and M. Batzill *Influence of Hydroxyls on Pd Atom Mobility and Clustering on Rutile TiO₂(011)-2 x 1* *ACS Nano*, 2014, 8 (6), pp 6321-6333 (<http://dx.doi.org/10.1021/nn501817w>)

- Developed for MC simulations of Pd on TiO₂ surfaces.

CHONSMgPNaFBLi-e.ff: (C/H/O/N/S/Mg/P/Na/F/B/Li/El/Ho) M.Islam and A.C.T van Duin *Reductive Decomposition Reactions of Ethylene Carbonate by Explicit Electron Transfer from Lithium: An eReaxFF Molecular Dynamics Study* *J. Phys. Chem. C*, 2016, 120 (48), pp 27128-27134 (<http://dx.doi.org/10.1021/acs.jpcc.6b08688>)

- This forcefield uses the ACKS2 charge model
- This forcefield is an eReaxFF forcefield
- Developed for the study of lithium-ion batteries
- NOTE: This ff uses vpar(38) for e-reaxff taper radius instead of vpar(41) that ADF-reaxff expects. This will generate a warning but should still work.

CHOFeAlNiCuScrSiGe.ff: (C/H/O/Fe/Al/Ni/Cu/S/Cr/Si/Ge) Y.Zheng, S. Hong, G. Psfogiannakis, S. Datta, B. Rayner, A.C.T. van Duin and R. Engel-Herbert *Modeling and In-situ Probing of Surface Reactions in Atomic Layer Deposition* *ACS Appl. Mater. Interfaces*, 2017, 9 (18), pp 15848-15856 (<http://dx.doi.org/10.1021/acsami.7b01618>)

- Used for studying the ALD process of Al₂O₃ from trimethylaluminum and water on hydrogenated and oxidized Ge(100) surfaces

Water2017.ff: (H/O/X) W.Zhang, A.C.T. van Duin *Second-Generation ReaxFF Water Force Field: Improvements in the Description of Water Density and OH-Anion Diffusion* *J. Phys. Chem. B*, 2017, 121 (24), pp 6021-6032 (<http://dx.doi.org/10.1021/acs.jpcc.7b02548>)

- Better description of liquid water

HSMo.ff: (H/S/Mo) A.Ostadossein, A. Rahnamoun, Y. Wang, P. Zhao, S. Zhang, V.H. Crespi, and A.C.T. van Duin *ReaxFF Reactive Force-Field Study of Molybdenum Disulfide (MoS₂)* *J. Phys. Chem. Lett.*, 2017, 8 (3), pp 631-640 (<http://dx.doi.org/10.1021/acs.jpclett.6b02902>)

- MoS₂ training set in supporting info
- strain-stress analysis

CHON2017_weak.ff: (C/H/O/N/S/Mg/P/Na/Cu/Cl/X) Weiwei Zhang and Adri C. T. van Duin *Improvement of the ReaxFF Description for Functionalized Hydrocarbon/Water Weak Interactions in the Condensed Phase* *J. Phys. Chem. B*, 2018, 122, 4083-4092 (<http://dx.doi.org/10.1021/acs.jpcc.8b01127>)

- retraining of the protein-2013 force-field (C, H, O, and N parameters for weak interactions)
- reproduces well the density of liquid water and hydrocarbons

CaSiOH.ff: (C/H/O/Ca/Si/X) Hegoi Manzano, Roland J. M. Pellenq, Franz-Josef Ulm, Markus J Buehler, and A.C.T. van Duin *Hydration of Calcium Oxide Surface Predicted by Reactive Force Field Molecular Dynamics* *Langmuir*, 2012, 28 (9), 4187-4197 (<http://dx.doi.org/10.1021/la204338m>)

- hydration of calcium oxide surface
- fitted using density functional theory calculations on gas phase calcium-water clusters, calcium oxide bulk and surface properties, calcium hydroxide, bcc and fcc Ca, and proton transfer reactions in the presence of calcium.

CHO-2016.ff: (C/H/O) Chowdhury Ashraf and Adri C.T. van Duin* *Extension of the ReaxFF Combustion Force Field toward Syngas Combustion and Initial Oxidation Kinetics* *J. Phys. Chem. A* 121, 5, 1051-1068 (<https://dx.doi.org/10.1021/acs.jpca.6b12429>)

- improved description of oxidation of small hydrocarbons and syngas reaction

CHON2017_weak_bb.ff: (C/H/O/N/S/Mg/P/Na/Cu/Cl/X) Vashisth A., Ashraf C., Zhang W., Bakis C.E., van Duin A.C.T. *Accelerated ReaxFF Simulations for Describing the Reactive Cross-Linking of Polymers* *J Phys Chem A*. 2018 Aug 1. (<https://doi.org/10.1021/acs.jpca.8b03826>)

- reparametrized version of CHON2017_weak.ff for bond-boost application

CH_aromatics.ff: (C/H) Qian Mao, Yihua Ren, K. H. Luo, Adri C. T. van Duin *Dynamics and kinetics of reversible homo-molecular dimerization of polycyclic aromatic hydrocarbons* *The Journal of Chemical Physics* 147, 244305 (2017) (<https://doi.org/10.1063/1.5000534>)

- ff for polycyclic aromatic hydrocarbons

CuSCH.ff: (C/H/O/S/Cu/Cl/X) Jejoon Yeon, H.L. Adams, C.E. Junkermeier, A.C.T. van Duin, W.T. Tysoe, and A. Martini *Development of a ReaxFF Force Field for Cu/S/C/H and Reactive MD Simulations of Methyl Thiolate Decomposition on Cu (100)* *J. Phys. Chem. B*, 2018, 122 (2), pp 888-896 (<https://doi.org/10.1021/acs.jpcc.7b06976>)

- combination of CuCl-H₂O.ff and AuSCH_2011.ff
- reparametrized Cu-S parameters with copper sulfides data

TiO₂bio.ff: (C/H/O/N/S/Mg/P/Na/Ti/Cl/F/X) Susanna Monti, Mariachiara Pastore, Cui Li, Filippo De Angelis, and Vincenzo Carravetta *Theoretical Investigation of Adsorption, Dynamics, Self-Aggregation, and Spectroscopic*

Properties of the D102 Indoline Dye on an Anatase (101) Substrate J. Phys. Chem. C, 2016, 120 (5), pp 2787–2796 (<https://doi.org/10.1021/acs.jpcc.5b11332>)

CHFe.ff: (C/H/Fe) Md Mahbubul Islam, Chenyu Zou, Adri C. T. van Duin and Sumathy Raman *Interactions of hydrogen with the iron and iron carbide interfaces: a ReaxFF molecular dynamics study* Phys. Chem. Chem. Phys., 2016, 18, 761-771 (<https://doi.org/10.1039/C5CP06108C>)

CHoGe.ff: (C/H/O/Ge) Nadire Nayir, Adri C.T. van Duin and Sakir Erkoç *Development of a ReaxFF Reactive Force Field for Interstitial Oxygen in Germanium and Its Application to GeO₂/Ge Interfaces* J. Phys. Chem. C, 2019, 123 (2), pp 1208–1218 (<http://dx.doi.org/10.1021/acs.jpcc.8b08862>)

- Created by extending the training set from CHoFeAlNiCuSCrSiGe.ff by Zheng et al. with additional crystal data
- Some general parameters were missing in the Supporting Information

CHONSSi.ff: (C/H/O/N/S/Si) F.A. Soria, W. Zhang, P.A. Paredes-Olivera, A.C.T. van Duin and E.M. Patrito *Si/C/H ReaxFF Reactive Potential for Silicon Surfaces Grafted with Organic Molecules* J. Phys. Chem. C, 2018, 122 (41), pp 23515-23527 (<http://dx.doi.org/10.1021/acs.jpcc.8b07075>)

- developed for the study of the functionalization and decomposition of alkyl monolayers on silicon surface

CHOSiNa.ff: (C/H/O/Si/Na) S.H. Hahn, J. Rimsza, L. Criscenti, Wei Sun, Lu Deng, Jincheng Du, Tao Liang, S.B. Sinnott, and A.C.T. van Duin *Development of a ReaxFF Reactive Force Field for NaSiO_x/Water Systems and Its Application to Sodium and Proton Self-Diffusion* J. Phys. Chem. C, 2018, 122 (34), pp 19613-19624 (<https://dx.doi.org/10.1021/acs.jpcc.8b05852>)

- developed for reactive MD simulation of the sodium silicate-water interfaces
- validated for sodium silicate crystal structures and glasses, and transport properties of sodium ions and protons within the amorphous structures

CHOCsKNaClIFLi.ff: (C/H/O/Cs/K/Na/Cl/I/F/Li) M.V. Fedkin, Y.K. Shin, N. Dasgupta, J. Yeon, W. Zhang, D. van Duin, A.C.T. van Duin, K. Mori, A. Fujiwara, M. Machida, H. Nakamura, and M. Okumura *Development of the ReaxFF Methodology for Electrolyte-Water Systems* J. Phys. Chem. A, 2019, 123 (10), pp 2125-2141 (<http://dx.doi.org/10.1021/acs.jpca.8b10453>)

- developed for water-electrolyte systems with Li⁺, Na⁺, K⁺, Cs⁺, F⁻, Cl⁻, and I⁻
- trained against (QM) calculations related to water binding energies, hydration energies and energies of proton transfer

INCLUDED FORCE FIELDS (DEVELOPMENT)

See also [Included force fields \(released version\)](#)

Description of ReaxFF force fields

Disclaimer: Using these forcefields for systems they have not been explicitly trained against may produce unrealistic results. Please see the full manuscripts for more detailed information.

The force field files used by the SCM version of ReaxFF are compatible with those used by the original ReaxFF code. So if you have the force field information from somewhere else you can just use it (save it in a text file, and select it in AMSinput via the Other... option).

There are currently two major groupings (i.e., the ReaxFF branches) of parameter sets that are intra-transferable with one another: (1) the combustion branch and (2) the aqueous (water) branch. The major difference between these two branches is in the O/H parameters, where the combustion branch focuses on accurately describing water as a gas-phase molecule, and the water branch is targeted at aqueous chemistry.

AB.ff: (H/O/N/B) Ammonia Borane M.R.Weismiller, A.C.T. van Duin, J. Lee, R.A. Yetter *ReaxFF Reactive Force Field Development and Applications for Molecular Dynamics Simulations of Ammonia Borane Dehydrogenation and Combustion* *J. Phys. Chem. A* 2010, 114, 5485-5492 (<http://dx.doi.org/10.1021/jp100136c>)

- QM data were generated describing the single and (if relevant) double and triple bond dissociation for all B/N/O/H combinations. These data were used to derive initial ReaxFF bond parameters, and all calculations were performed using DFT with the B3LYP functional and the Pople 6-311G** basis set.
- The training set was then extended with QM data describing angular distortions in a set of small AB-related (AB H₃N-BH₃) molecules. These data were used to derive the initial ReaxFF angular parameters.
- The training set was extended with reaction barriers for key reaction steps such as H₂ release from AB, dimerization of H₂B-NH₂ and reaction energies associated with H₂ release from AB and with AB oxidation.
- Branch: combustion.

AuCSOH.ff: (Au/C/S/O/H) J.A. Keith, D. Fantauzzi, T. Jacob, and A.C.T. van Duin *Reactive forcefield for simulating gold surfaces and nanoparticles* *Physical Review B* (2010) 81, 235404-1/235404-8 (<http://dx.doi.org/10.1103/PhysRevB.81.235404>)

- The original Au-Au parameters were extended by three publications:
- Au/O: K. Joshi, A.C.T. van Duin, and T. Jacob Development of a ReaxFF description of gold oxides and initial application to cold welding of partially oxidized gold surfaces *Journal of Materials Chemistry* 20, (2010), 10431-10437 <http://dx.doi.org/10.1039/C0JM01556C>
- Au/C/S/H: T.T. Jarvi, A.C.T. van Duin, K. Nordlund, and W.A. Goddard Development of interatomic ReaxFF potentials for Au-S-C-H systems *Journal of Physical Chemistry C* 115, (2011), 10315-10322 <http://dx.doi.org/10.1021/jp201496x>

- C/O/H/S: Rahaman, O., van Duin, A. C. T., Goddard, W. A., III, and Doren, D. J. Development of a ReaxFF reactive force field for glycine and application to solvent effect and tautomerization *Journal of Physical Chemistry B* 115 (2011), 249-261 <http://dx.doi.org/10.1021/jp108642r>
- The forcefield does not include Au/N parameters
- Branch: water.

CHO.ff: (C/H/O) Hydrocarbon oxidation K.Chenoweth, A.C.T. van Duin, W. A. Goddard *ReaxFF Reactive Force Field for Molecular Dynamics Simulations of Hydrocarbon Oxidation* *J. Phys. Chem. A* 2008, 112, 1040-1053 (<http://dx.doi.org/10.1021/jp709896w>)

- To obtain the H/C/O compound data required to extend the hydrocarbon-training set, DFT calculations were performed on the following systems: (a) dissociation energies for various bonds containing carbon, oxygen, and hydrogen. The ground state structure was obtained through full geometry optimization. Dissociation curves were calculated by constraining only the bond length of interest and re-optimization of the remaining internal coordinates. Optimization was also performed for the various angles and torsions associated with C/H/O interactions.
- Branch: combustion.

HCONSB.ff: (H/C/O/N/S/B) M.R. Weismiller, A.C.T. van Duin, J. Lee, and R.A. Yetter, *ReaxFF Reactive Force Field Development and Applications for Molecular Dynamics Simulations of Ammonia Borane Dehydrogenation and Combustion* *J. Phys. Chem. A* (2010), 114, 5485-5492. (<http://dx.doi.org/10.1021/jp100136c>)

- The parameters in this forcefield were extended/improved by two other publications:
- A.M. Kamat, A.C.T. van Duin, and A. Yakovlev *Molecular Dynamics Simulations of Laser-Induced Incandescence of Soot Using an Extended ReaxFF Reactive Force Field*. *Journal of Physical Chemistry A* (2010), 114, 12561-1257 <http://dx.doi.org/10.1021/jp1080302>
- F.Castro-Marcano, A.M. Kamat, M.F. Russo, A.C.T. van Duin, and J.P. Mathews *Combustion of an Illinois No. 6 Coal Char Simulated Using an Atomistic Char Representation and the ReaxFF Reactive Force Field*. *Combustion and Flame* (2012), 159, 23273-1285 <http://dx.doi.org/10.1016/j.combustflame.2011.10.022>
- The C/H/O parameters are the same as in the CHO forcefield, with added S/C, S/H and S/O descriptions. This force field was used in Castro et al, *Combustion and Flame* 2011
- The Boron and Nitrogen parameters are based on (but not identical to) the parameters used in Weismiller et al, *JPC-A* 2010.
- Branch: combustion.

CuCl-H2O.ff: (Cu/Cl/H/O) O.Rahaman, A.C.T. van Duin, V.S. Bryantsev, J.E. Mueller, S.D. Solares, W.A. Goddard III, and D.J. Doren *Development of a ReaxFF Reactive Force Field for Aqueous Chloride and Copper Chloride* *J. Phys. Chem. A* 114 (2010), 3556-3568 (<http://dx.doi.org/10.1021/jp9090415>)

- This forcefield is an extension of: A.C.T. van Duin, V.S. Bryantsev, M.S. Diallo, W.A. Goddard, O. Rahaman, D.J. Doren, D. Raymand, and K. Hermansson *Development and validation of a ReaxFF reactive force field for Cu cation/water interactions and copper metal/metal oxide/metal hydroxide condensed phases* *Journal of Physical Chemistry A* 2010, 114, 9507-9514 <http://dx.doi.org/10.1021/jp102272z>
- Branch: water.

FeOCHCl.ff: (Fe/O/C/H/Cl) M.Aryanpour, A.C.T. van Duin, J.D. Kubicki *Development of a Reactive Force Field for Iron-Oxyhydroxide Systems* *J. Phys. Chem. A* 2010, 114, 6298-6307 (<http://dx.doi.org/10.1021/jp101332k>)

- The Cl parameters were published by: O. Rahaman, A.C.T. van Duin, V.S. Bryantsev, J.E. Mueller, S.D. Solares, W.A. Goddard III, and D.J. Doren *Development of a ReaxFF Reactive Force Field for Aqueous Chloride and Copper Chloride* *J. Phys. Chem. A* 114 (2010), 3556-3568 <http://dx.doi.org/10.1021/jp9090415>

- The initial force field parameters for the Fe-Fe parameters were taken from an earlier force field development project on bulk-iron metal, based on DFT-calculations on antiferromagnetic BCC and FCC. The ReaxFF parameters have not been published yet, however the DFT data can be found in ref 31 of the above mentioned manuscript. The O/H parameters were taken from the ReaxFF bulk water description. The Fe/Fe and O/H parameters were kept fixed to these initial values, whereas the Fe/O parameters were reoptimized against the quantum mechanical results presented in the above mentioned manuscript.
- Detailed information on the force field parameters is given in the supporting information of the above mentioned manuscript.
- Branch: water.

HE.ff: (C/H/O/N) RDX/High Energy L.Z. Zhang, A.C.T. van Duin, S.V. Zybin, and W.A. Goddard *Thermal Decomposition of Hydrazines from Reactive Dynamics Using the ReaxFF Reactive Force Field* *Journal of Physical Chemistry B* (2009) 113, 10770-10778 (<http://dx.doi.org/10.1021/jp900194d>)

- Part of this forcefield is also published in: L.Z. Zhang, S.V. Zybin, A.C.T. van Duin, S. Dasgupta, W.A. Goddard, and E.M. Kober *Carbon Cluster Formation during Thermal Decomposition of Octahydro-1,3,5,7-tetranitro-1,3,5,7-tetrazocine and 1,3,5-Triamino-2,4,6-trinitrobenzene High Explosives from ReaxFF Reactive Molecular Dynamics Simulations* *Journal of Physical Chemistry A* (2009) 113, 10619-10640 <http://dx.doi.org/10.1021/jp901353a>
- The parameters of the nitramine ReaxFF are based on a large number of ab initio QM calculations. Over 40 reactions and over 1600 equilibrated molecules have been used; they are designed to characterize the atomic interactions under various environments likely and unlikely high energy each atom can encounter. The training set contains bond breaking and compression curves for all possible bonds, angle and torsion bending data for all possible cases, as well as crystal data.
- Please see the supplemental material from *Phys. Rev. Lett.* 2003, 91, 098301 for a detailed description of the parameterization of this force field.
- Branch: combustion.

HE2.ff: (C/H/O/N/S/Si) RDX/High Energy L.Z. Zhang, S.V. Zybin, A.C.T. van Duin, S. Dasgupta, W.A. Goddard, and E.M. Kober *Carbon Cluster Formation during Thermal Decomposition of Octahydro-1,3,5,7-tetranitro-1,3,5,7-tetrazocine and 1,3,5-Triamino-2,4,6-trinitrobenzene High Explosives from ReaxFF Reactive Molecular Dynamics Simulations* *Journal of Physical Chemistry A* (2009) 113, 10619-10640 (<http://dx.doi.org/10.1021/jp901353a>)

- Similar to HE.ff with additional parameters fitted for the TATB explosive
- Branch: combustion.

NaH.ff: (Na/H) J.G.O. Ojwang, R. Van Santen, G.J. Kramer, A.C.T. van Duin, and W.A. Goddard *Modeling the sorption dynamics of NaH using a reactive force field* *Journal of Chemical Physics* 2008, 128, 164714 (<http://dx.doi.org/10.1063/1.2908737>)

- This forcefield originally had a typo, defining the H-Na-Na angle twice. The same typo is in table 4 of the publication, but the text clearly mentions that the second line should define Na-H-Na instead.
- Branch: combustion.

NiCH.ff: (Ni/C/H) J.E. Mueller, A.C.T. van Duin, and W.A. Goddard III *Development and Validation of ReaxFF Reactive Force Field for Hydrocarbon Chemistry Catalyzed by Nickel* *J. Phys. Chem. C* 2010, 114, 4939-4949 (<http://dx.doi.org/10.1021/jp9035056>)

- Branch: combustion.

SiOH.ff: (Si/O/H) J.C. Fogarty, H.M. Aktulga, A.Y. Grama, A.C.T. van Duin, S.A. Pandit *A reactive molecular dynamics simulation of the silica-water interface* *J. Chem. Phys.* 2010, 132, 174704 (<http://dx.doi.org/10.1063/1.3407433>)

- This force field was trained to model the interaction of water at the SiO₂ surface, with specific emphasis on proton-transfer reactions. Updated parameters were fitted for all Si/O/H bond, angle, and torsion interactions as well, in addition to the dissociation of a water molecule from a single Si(OH)₄ molecule and reaction energies for the polymerization of Si(OH)₄
- Branch: water.

SiC.ff: (Si/C/O/H/N/S) D.Newsome, D. Sengupta, H. Foroutan, M.F. Russo, and A.C.T. van Duin *Oxidation of Silicon Carbide by O₂ and H₂O: A ReaxFF Reactive Molecular Dynamics Study, Part I* *Journal of Physical Chemistry* 2012 116, 16111-16121 (<http://dx.doi.org/10.1021/jp306391p>)

- The included forcefield is based on the Newsome reference, with slightly improved parameters by van Duin et al.
- Branch: combustion.

VOCH.ff: (V/O/C/H) K.Chenoweth, A.C.T. van Duin, P. Persson, M.J. Cheng, J. Oxgaard, W.A. Goddard *Development and Application of a ReaxFF Reactive Force Field for Oxidative Dehydrogenation on Vanadium Oxide Catalysts* *J. Phys. Chem. C*, 2008, 112, 14645-14654 (<http://dx.doi.org/10.1021/jp802134x>)

- The ReaxFF force field parameters have been fit to a large quantum mechanics (QM) training set containing over 700 structures and energetics related to bond dissociations, angle and dihedral distortions, and reactions between hydrocarbons and vanadium oxide clusters. In addition, the training set contains charge distributions for small vanadium oxide clusters and the stabilities of condensed-phase systems including V₂O₅, VO₂, and V₂O₃ in addition to metallic V (V₀).
- Branch: combustion.

ZnOH.ff: (Zn/O/H) D.Raymand, A.C.T. van Duin, M. Baudin, K. Hermansson *A reactive force field (ReaxFF) for zinc oxide* *Surface Science* 2008, 602, 1020-1031 (<http://dx.doi.org/10.1016/j.susc.2007.12.023>)

- updated version published by: D. Raymand, A.C.T. van Duin, D. Spangberg, W.A. Goddard, K. Hermansson *Water adsorption on stepped ZnO surfaces from MD simulation* *Surface Science* 2010, 604, 9-10, 741-752 <http://dx.doi.org/10.1016/j.susc.2009.12.012>
- Based on QM calculations for Zn(s), ZnO(s), and Zn hydroxide clusters [Zn(OH)₂ and O(ZnOH)₂], ReaxFF parameters were generated for Zn-O and Zn-Zn bond energies and for Zn-O-Zn, O-Zn-O, O-Zn-Zn and Zn-O-H valence angle energies.
- QM calculations were performed for the four crystal polymorphs of the wurtzite, zincblende, rocksalt and caesium chloride structures (the structures are also referred to as h-ZnS, c-ZnS, NaCl and CsCl, respectively).
- Branch: water.

Al-H₂O.ff: (Al/H/O) M.Russo, R. Li, M. Mench, and A.C.T. van Duin *Molecular Dynamic Simulation of Aluminum-Water Reactions Using the ReaxFF Reactive Force Field* *International Journal of Hydrogen Energy* 36 (2011), 5828-5835 (<http://dx.doi.org/10.1016/j.ijhydene.2011.02.035>)

- Branch: water.

CaSiAlO.ff: (C/H/O/Fe/Cl/Si/Al/Ca) M.C. Pitman and A.C.T. van Duin *Dynamics of Confined Reactive Water in Smectite Clay-Zeolite Composites* *J. Am. Chem. Soc.*, 2012, 134 (6), 3042-3053 (<http://dx.doi.org/10.1021/ja208894m>)

- Branch: water.

dispersion/CHONSSi-Ig.ff: (C/H/O/N/S/Si) L.Liu, Y. Liu, S.V. Zybin, H. Sun, and W.A. Goddard III *ReaxFF-Ig: Correction of the ReaxFF Reactive Force Field for London Dispersion, with Applications to the Equations of State for Energetic Materials* *The Journal of Physical Chemistry A*, 2011, 115(40), 11016-11022 (<http://dx.doi.org/10.1021/jp201599t>)

- This forcefield adds London dispersion correction terms to reaxFF, and is optimized for the energetic materials RDX, PETN, TATB, and NM plus graphite, polyethylene, solid carbon dioxide, and solid N₂, using the low temperature crystal structures to determine the lg correction parameters.
- Branch: combustion.

CHOFeAlNiCuS.ff: (C/H/O/Fe/Al/Ni/Cu/S) O.Rahaman, A.C.T. van Duin, W.A. Goddard III, and D.J. Doren *Development of a ReaxFF reactive force field for glycine and application to solvent effect and tautomerization* *Journal of Physical Chemistry B* 115 (2011), 249-261. (<http://dx.doi.org/10.1021/jp204894m>)

- C/O/H parameters only. The Cu/Fe/Al/Ni parameters are from: Y.K. Shin, H. Kwak, C. Zou, A.V. Vasenkov, and A.C.T. van Duin *Development and Validation of a ReaxFF Reactive Force Field for Fe/Al/Ni Alloys: Molecular Dynamics Study of Elastic Constants, Diffusion, and Segregation* *J. Phys. Chem. A*, 2012, 116 (49), pp 12163–12174 <http://dx.doi.org/10.1021/jp308507x>
- Not all cross-terms between the two forcefield files are defined, which might cause problems if the system has (for example) C-Cu interactions.
- Branch: water.

AuSCH_2011.ff: (Au/S/C/H) T.T. Jarvi, A.C.T. van Duin, K. Nordlund, and W.A. Goddard III, *Development of Interatomic ReaxFF Potentials for Au-S-C-H Systems* *J. Phys. Chem. A*, 115, 10315-10322 (2011) (<http://dx.doi.org/10.1021/jp201496x>)

- Branch: combustion.

AuSCH_2013.ff: (Au/S/C/H) Gyun-Tack Bae and Christine M. Aikens *Improved ReaxFF Force Field Parameters for Au-S-C-H Systems* *Journal of Physical Chemistry A* 2013 117 (40), 10438-10446 (<http://dx.doi.org/10.1021/jp405992m>)

- Based upon: T.T. Jarvi, A.C.T. van Duin, K. Nordlund, and W.A. Goddard *Development of interatomic ReaxFF potentials for Au-S-C-H systems*. *Journal of Physical Chemistry C* 115, (2011), 10315-10322.
- yields improvements for bond bending potential energy surfaces
- aims to agree with DFT geometries of small clusters and gold-thiolate nanoparticles
- Branch: combustion.

PDMSDecomp.ff: (C/H/O/Si) K.Chenoweth, S. Cheung, A.C.T. van Duin, W.A. Goddard III, and E.M. Kober *Simulations on the Thermal Decomposition of a Poly(dimethylsiloxane) Polymer Using the ReaxFF Reactive Force Field* *J. Am. Chem. Soc.*, 2005, 127 (19), pp 7192-7202 (<http://dx.doi.org/10.1021/ja050980t>)

- Specialized forcefield, designed to “investigate the failure of the poly(dimethylsiloxane) polymer (PDMS) at high temperatures and pressures and in the presence of various additives”
- Line from the torsion block was referring to non-existent atoms from the atomic block and thus was removed.
- Branch: combustion.

TiOCHNCl.ff: (C/H/O/N/S/Mg/P/Na/Ti/Cl/F) S.Y. Kim, A.C.T. van Duin, and J.D. Kubicki *Molecular dynamics simulations of the interactions between TiO₂ nanoparticles and water with Na⁺ and Cl⁻, methanol, and formic acid using a reactive force field* *Journal of Materials Research / Volume 28 / Issue 03 / 2013*, pp 513-520 (<http://dx.doi.org/10.1557/jmr.2012.367>)

- used for simulating TiO₂(both rutile and anatase) nanoparticles with water, methanol, and formic acid
- The force field was validated by comparing water dissociative adsorption percentage and bond length between Na-O with density functional theory (DFT) and experimental results
- Branch: water.

PtCH.ff: (C/H/Pt) C.F. Sanz-Navarro, P. Astrand, De Chen, M. Ronning, A.C.T. van Duin, T. Jacob, and W.A. Goddard III *Molecular Dynamics Simulations of the Interactions between Platinum Clusters and Carbon Platelets* J. Phys. Chem. A 112, 1392-1402 (2008) (<http://dx.doi.org/10.1021/jp074806y>)

- Branch: combustion.

BaYZrCHO.ff: (C/H/O/Ba/Zr/Y) A.C.T. van Duin, B.V. Merinov, S.S. Jang, and W.A. Goddard III *ReaxFF Reactive Force Field for Solid Oxide Fuel Cell Systems with Application to Oxygen Ion Transport in Yttria-Stabilized Zirconia* J. Phys. Chem. A, 112, 3133-3140 (2008) (<http://dx.doi.org/10.1021/jp076775c>)

- Branch: combustion.

CHONSSiPtZrNiCuCo.ff: (C/H/O/N/S/Si/Pt/Zr/Ni/Cu/Co) K.D. Nielson, A.C.T. van Duin, J. Oxgaard, W.Q. Deng, and W.A. Goddard III *Development of the ReaxFF Reactive Force Field for Describing Transition Metal Catalyzed Reactions, with Application to the Initial Stages of the Catalytic Formation of Carbon Nanotubes* J. Phys. Chem. A, 109, 493-499 (2005) (<http://dx.doi.org/10.1021/jp046244d>)

- Branch: combustion.

Glycine.ff: (C/H/O/N) O.Rahaman, A.C.T. van Duin, W.A. Goddard III, and D.J. Doren, *Development of a ReaxFF Reactive Force Field for Glycine and Application to Solvent Effect and Tautomerization* J. Phys. Chem. B, 115, 249-261 (2011) (<http://dx.doi.org/10.1021/jp108642r>)

- Line from the valence angle block was referring to non-existent atoms from the atomic block and thus was removed.
- Branch: water.

SiONH.ff: (C/H/O/N/Si/S) A.D. Kulkarni, D.G. Truhlar, S.G. Srinivasan, A.C.T. van Duin, P. Norman, and T.E. Schwartztruber *Oxygen Interactions with Silica Surfaces: Coupled Cluster and Density Functional Investigation and the Development of a New ReaxFF Potential* J. Phys. Chem. C, 2013, 117 (1), pp 258-269 (<http://dx.doi.org/10.1021/jp3086649>)

- Aimed at oxygen interactions with realistic silica surfaces
- Lines from the valence angle block was referring to non-existent atoms from the atomic block and thus was removed.
- Branch: combustion.

CHOFe.ff: (C/H/O/Fe/Cl/Si/Al) Chenyu Zou, A.C.T. Van Duin *Investigation of Complex Iron Surface Catalytic Chemistry Using the ReaxFF Reactive Force Field Method* JOM, December 2012, Volume 64, Issue 12, pp 1426-1437 (<http://dx.doi.org/10.1007/s11837-012-0463-5>)

- only the parameters for Fe (and crossterms) differ from the CHOAlSi.ff forcefield
- Branch: water.

CHOAlSi.ff: (C/H/O/Fe/Cl/Si/Al) F.Castro-Marcanao, A.C.T. van Duin *Comparison of thermal and catalytic cracking of 1-heptene from ReaxFF reactive molecular dynamics simulations* Combustion and Flame, Volume 160, Issue 4, April 2013, Pages 766-775 (<http://dx.doi.org/10.1016/j.combustflame.2012.12.007>)

- only the parameters for Fe (and crossterms) differ from the CHOFe.ff forcefield
- Branch: water.

CHOLi.ff: (C/H/O/N/S/Mg/P/Na/Li) D.Bedrov, G.D. Smith, A.C.T. van Duin *Reactions of Singly-Reduced Ethylene Carbonate in Lithium Battery Electrolytes: A Molecular Dynamics Simulation Study Using the ReaxFF* Journal of Physical Chemistry A, 2012, 116 (11), pp 2978-2985 (<http://dx.doi.org/10.1021/jp210345b>)

- specifically generated for simulating Lithium battery electrolytes
- must be used in combination with the MOLCHARGE keyword to set a charge restraint on Li and CO3!
- Branch: water.

SiOAlLi.ff: (H/O/Si/Al/Li) B.Narayanan, A.C.T. van Duin, B.B. Kappes, I.E. Reimanis and C.V. Ciobanu *A reactive force field for lithium-aluminum silicates with applications to eucryptite phases* *Modelling and Simulation in Materials Science and Engineering* 2012 20 015002 (<http://dx.doi.org/10.1088/0965-0393/20/1/015002>)

- Branch: water.

PdO.ff: (Pd/O) T.P. Senftle, R.J. Meyer, M.J. Janik and A.C.T. van Duin *Development of a ReaxFF potential for Pd/O and application to palladium oxide formation* *The Journal of Chemical Physics* 139, 044109 (2013) (<http://dx.doi.org/10.1063/1.4815820>)

- used for studying Oxidation states of Pd nanoparticles, surfaces and bulk configurations with a GCMC method
- Branch: combustion.

PdH.ff: (Pd/H) T.P. Senftle, M.J. Janik and A.C.T. van Duin *A ReaxFF Investigation of Hydride Formation in Palladium Nanoclusters via Monte Carlo and Molecular Dynamics Simulations* *The Journal of Physical Chemistry C*, 2014, 118 (9), pp 4967-4981 (<http://dx.doi.org/10.1021/jp411015a>)

- used in combination with a GCMC method
- Branch: combustion.

Co.ff: (Co) Xue-Qing Zhang, E. Iype, S.V. Nedeia, A.P.J. Jansen, B.M. Szyja, E.J.M. Hensen, and R.A. van Santen *Site Stability on Cobalt Nanoparticles: A Molecular Dynamics ReaxFF Reactive Force Field Study* *The Journal of Physical Chemistry C*, 2014, 118 (13), pp 6882-6886 (<http://dx.doi.org/10.1021/jp500053u>)

- forcefield was generated using a recently developed Monte Carlo algorithm with simulated annealing.
- Branch: combustion.

CHONSMgPNaCuCl.ff: (C/H/O/N/S/Mg/P/Na/Cu/Cl) Susanna Monti, Cui Li, and Vincenzo Carravetta *Reactive Dynamics Simulation of Monolayer and Multilayer Adsorption of Glycine on Cu(110)* *J. Phys. Chem. C*, 2013, 117 (10), pp 5221-5228 (<http://dx.doi.org/10.1021/jp312828d>)

- Reactive MD-force field for amino acids on copper
- Branch: water.

CHOSMoNiLiBFPN.ff: (C/H/O/S/Mo/Ni/Li/B/F/P/N) Md M. Islam, V.S. Bryantsev, A.C.T. van Duin *ReaxFF Reactive Force Field Simulations on the Influence of Teflon on Electrolyte Decomposition during Li/SWCNT Anode Discharge in Lithium-Sulfur Batteries* *J. Electrochem. Soc.* 2014 volume 161, issue 8, E3009-E3014 (<http://dx.doi.org/10.1149/2.005408jes>)

- forcefield for Electrochemistry in Li-S batteries
- Branch: combustion.

CHONSSiNaFZr.ff: (C/H/O/N/S/Si/Na/F/Zr) A.Rahnamoun and A.C.T. van Duin *Reactive Molecular Dynamics Simulation on the Disintegration of Kapton, POSS Polyimide, Amorphous Silica, and Teflon during Atomic Oxygen Impact Using the Reaxff Reactive Force-Field Method* *J. Phys. Chem. A*, 2014, 118 (15), pp 2780-2787 (<http://dx.doi.org/10.1021/jp4121029>)

- comments in the forcefield file: interactions with water and Na+ Fogarty et al. JCP-2010 ; with glycine + C/H/F parameters; Si-F bond/offdiag/angle parameters; Si-S dummy parameters + S-O-H parameters(Yun 2012 Oct8) + H-F bond/offdiag (Jan14 2013 Joon) Jan31: added Zr/O/H/C
- Branch: water.

TiClOH.ff: (C/H/O/N/S/Mg/P/Na/Ti/Cl/F) Sung-Yup Kim and A.C.T. van Duin *Simulation of Titanium Metal/Titanium Dioxide Etching with Chlorine and Hydrogen Chloride Gases Using the ReaxFF Reactive Force Field* *J. Phys. Chem. A*, 2013, 117 (27), pp 5655-5663 (<http://dx.doi.org/10.1021/jp4031943>)

- adaptation/evolution of the TiOCHNCl.ff forcefield by Kim, S.-Y. et al.

- Branch: water.

CHONSSiNaAl.ff: (C/H/O/N/S/Si/Na/Al) C.Bai, L. Liu, and H. Sun *Molecular Dynamics Simulations of Methanol to Olefin Reactions in HZSM-5 Zeolite Using a ReaxFF Force Field* *J. Phys. Chem. C*, 2012, 116 (12), pp 7029-7039 (<http://dx.doi.org/10.1021/jp300221j>)

- used to simulate methanol to olefin (MTO) reactions in H-ZSM-5 zeolite
- Branch: water.

undocumented/NiCH.ff: (Ni/C/H/O/N/S/F/Pt/Cl) Unknown *No Name* Not published (<http://>)

- This forcefield is from april 2009, and is not published
- Branch: combustion.

LiS.ff: (Li/S) Md M. Islam, A. Ostadhossein, O. Borodin, A.T. Yeates, W.W. Tipton, R.G. Hennig, N. Kumar, and A.C.T. van Duin *ReaxFF molecular dynamics simulations on lithiated sulfur cathode materials* *Phys. Chem. Chem. Phys.*, 2015, 17, 3383-3393 (<http://dx.doi.org/10.1039/C4CP04532G>)

- Developed for and used to study Sulfur cathode behaviour in Li battery cells
- Branch: combustion.

CHONSSiPtNiCuCoZrYBa.ff: (C/H/O/N/S/Si/Pt/Ni/Cu/Co/Zr/Y/Ba) B.V. Merinov, J.E. Mueller, A.C.T. van Duin, Qi An, and W.A. Goddard III *ReaxFF Reactive Force-Field Modeling of the Triple-Phase Boundary in a Solid Oxide Fuel Cell* *J. Phys. Chem. Lett.*, 2014, 5 (22), pp 4039-4043 (<http://dx.doi.org/10.1021/jz501891y>)

- Force field was developed by combining the YSZ and Ni/C/H descriptions
- From the summary: “The products obtained in our simulations are the same as those in experiment, which indicates that the developed ReaxFF potential properly describes complex physicochemical processes, such as the oxide-ion diffusion, fuel conversion, water formation reaction, coking, and delamination, occurring at the TPB and can be recommended for further computational studies of the fuel/electrode/electrolyte interfaces in a SOFC”
- The Aa atom type is a rename of the Zr atom type, which was defined twice.
- Branch: combustion.

CHONSSiNaP.ff: (C/H/O/N/S/Si/Na/P) Bo Zhang, A.C.T. van Duin and J.K. Johnson *Development of a ReaxFF Reactive Force Field for Tetrabutylphosphonium Glycinate/CO₂ Mixtures* *J. Phys. Chem. B*, 2014, 118 (41), pp 12008-12016 (<http://dx.doi.org/10.1021/jp5054277>)

- The forcefield file mentions “Gly with dummy N-P parameters”
- It was developed for studying Carbon dioxide interactions with the ionic liquid tetrabutylphosphonium glycinate, both physical and chemical absorption.
- Several lines from valence angle block were referring to non-existent atoms from the atomic block and thus were removed.
- Branch: combustion.

CHOLi_2.ff: (C/H/O/Li) M.Raju, P. Ganesh, P.R.C. Kent, and A.C.T. van Duin *Reactive Force Field Study of Li/C Systems for Electrical Energy Storage* *J. Chem. Theory Comput.*, 2015, 11 (5), pp 2156-2166 (<http://dx.doi.org/10.1021/ct501027v>)

- Used for studying Li/C systems with GCMC and MD
- Also contains parameters for “Vi” and “GI”, but these virtual elements are not mentioned in the paper
- Parameters were fitted using a training set consisting, amongst others, of Li binding energies on pristine graphene and graphite, Li migration pathways in graphite and Li dissociation pathways in different hydrocarbons

- The forcefield was validated by a side-by-side comparison of ReaxFF and DFT energies for Li binding on a divacancy, and ReaxFF and DFT ground-state configurations for stage II and stage I stacking in graphite obtained using GCMC simulations
- The forcefield reproduces the in-plane Li ordering as well as the graphite stacking sequence for stage II and stage I compounds
- Branch: water.

CHONSiCaCsKSrNaMgAlCu.ff: (C/H/O/N/S/Si/Ca/Cs/K/Sr/Na/Mg/Al/Cu) G.M. Psfogiannakis, J.F. McCleerey, E. Jaramillo and A.C.T. van Duin *ReaxFF Reactive Molecular Dynamics Simulation of the Hydration of Cu-SSZ-13 Zeolite and the Formation of Cu Dimers* *J. Phys. Chem. C*, 2015, 119 (12), pp 6678-6686 (<http://dx.doi.org/10.1021/acs.jpcc.5b00699>)

- This Cu/Si/Al/O/H forcefield was developed for and used in MD simulations of the hydration of Cu-exchanged SSZ-13 catalyst.
- The force field was developed by merging and expanding previously tested and published ReaxFF force fields for Si/Al/O/H systems and Cu/O/H systems (citations 19-26 of the publication)
- This forcefield is an extension of K.L. Joshi et al 2014, <http://dx.doi.org/10.1039/C4CP02612H>, all non-Cu parameters are the same.
- Branch: water.

HOSMg.ff: (H/O/S/Mg) E.Iype, M. Hütter, A.P.J. Jansen, S.V. Nedeia and C.C.M. Rindt *Parameterization of a reactive force field using a Monte Carlo algorithm* *J. Comput. Chem.*, 2013, 34: 1143-1154 (<http://dx.doi.org/10.1002/jcc.23246>)

- This forcefield is optimized with a metropolis Monte-Carlo algorithm with simulated annealing to search for the optimum parameters for the ReaxFF force field in a high-dimensional parameter space.
- The optimization is done against a set of quantum chemical data for MgSO₄ hydrates.
- Branch: combustion.

CHONSMgPNaCuCl_v2.ff: (C/H/O/N/S/Mg/P/Na/Cu/Cl) S.Monti, A. Corozzi, P. Fristrup, K.L. Joshi, Yun Kyung Shin, P. Oelschlaeger, A.C.T. van Duin and V. Baronee *Exploring the conformational and reactive dynamics of biomolecules in solution using an extended version of the glycine reactive force field* *Phys. Chem. Chem. Phys.*, 2013, 15, 15062-15077 (<http://dx.doi.org/10.1039/C3CP51931G>)

- This forcefield is an extension of CHONSMgPNaCuCl.ff by S. Monti et al., *J. Phys. Chem. C*, 2013, 117 (10), pp 5221-5228, <http://dx.doi.org/10.1021/jp312828d>
- Developed for peptide and protein simulations
- Branch: water.

OPt.ff: (O/Pt) D.Fantauzzi, J. Bandlow, L. Sabo, J.E. Mueller, A.C.T. van Duin and T. Jacob *Development of a ReaxFF potential for Pt-O systems describing the energetics and dynamics of Pt-oxide formation* *Phys. Chem. Chem. Phys.*, 2014, 16, 23118-23133 (<http://dx.doi.org/10.1039/C4CP03111C>)

- Pt-Pt parameters for bulk platinum phases, low & high-index platinum surfaces and nanoclusters.
- O-Pt parameters for bulk platinum oxides, as well as oxygen adsorption and oxide formation on Pt(111) terraces and the {111} and {100} steps connecting them.
- Branch: combustion.

CHONSMgPNaTiClF.ff: (C/H/O/N/S/Mg/P/Na/Ti/Cl/F) Stijn Huygh, Annemie Bogaerts, Adri C.T. van Duin and Erik C. Neyts *Development of a ReaxFF reactive force field for intrinsic point defects in titanium dioxide* *Computational Materials Science*, Volume 95, December 2014, Pages 579-591, ISSN 0927-0256 (<http://dx.doi.org/10.1016/j.commatsci.2014.07.056>)

- Forcefield developed for studying the influence of intrinsic point defects on the chemistry with TiO₂ condensed phases.
- Forcefield seems to be based on TiOCHNCl.ff, <http://dx.doi.org/10.1557/jmr.2012.367>
- Branch: water.

LiSi.ff: (Li/Si) A.Ostadossein, E.D. Cubuk, G.A. Tritsarlis, E. Kaxiras, S. Zhanga and A.C.T. van Duin *Stress effects on the initial lithiation of crystalline silicon nanowires: reactive molecular dynamics simulations using ReaxFF* Phys. Chem. Chem. Phys., 2015, 17, 3832-3840 (<http://dx.doi.org/10.1039/C4CP05198J>)

- Branch: combustion.

CHOFeAlNiCuSCr.ff: (C/H/O/Fe/Al/Ni/Cu/S/Cr) Y.K. Shin, H. Kwak, A.V. Vasenkov, D. Sengupta and A.C.T. van Duin *Development of a ReaxFF Reactive Force Field for Fe/Cr/O/S and Application to Oxidation of Butane over a Pyrite-Covered Cr₂O₃ Catalyst* ACS Catalysis, 2015, 5 (12), pp 7226-7236 (<http://dx.doi.org/10.1021/acscatal.5b01766>)

- Forcefield optimized for Fe/Cr/O/S
- Branch: water.

CHOFeAlNiCuSCr_v2.ff: (C/H/O/Fe/Al/Ni/Cu/S/Cr) Ni-O-vacancy C.Zou et al. *Molecular dynamics simulations of the effects of vacancies on nickel self-diffusion, oxygen diffusion and oxidation initiation in nickel, using the ReaxFF reactive force field* Acta Materialia, Volume 83, 15 January 2015, Pages 102-112 (<http://dx.doi.org/10.1016/j.actamat.2014.09.047>)

- Forcefield optimized for Ni/O, trained with a QM data on Ni, NiO and vacancies
- The non-carbon parameters are the same as in CHOFeAlNiCuSCr_v3.ff
- Branch: water.

CHOFeAlNiCuSCr_v3.ff: (C/H/O/Fe/Al/Ni/Cu/S/Cr) F.Tavazza, T.P. Senftle, C. Zou, C.A. Becker and A.C.T van Duin *Molecular Dynamics Investigation of the Effects of Tip-Substrate Interactions during Nanoindentation* J. Phys. Chem. C, 2015, 119 (24), pp 13580-13589 (<http://dx.doi.org/10.1021/acs.jpcc.5b01275>)

- Combination of the C.ff (condensed carbon) forcefield with Ni/C/O/H parameters
- The non-carbon parameters are the same as in CHOFeAlNiCuSCr_v2.ff
- Branch: water.

C.ff: (C) C-2013 S.G. Srinivasan, A.C.T. van Duin and P. Ganesh *Development of a ReaxFF Potential for Carbon Condensed Phases and Its Application to the Thermal Fragmentation of a Large Fullerene* J. Phys. Chem. A, 2015, 119 (4), pp 571-580 (<http://dx.doi.org/10.1021/jp510274e>)

- Forcefield designed for modeling Carbon condensed phases
- Branch: combustion.

CHONSSiGe.ff: (C/H/O/N/S/Si/Ge) G.Psofogiannakis and A.C.T van Duin *Development of a ReaxFF reactive force field for Si/Ge/H systems and application to atomic hydrogen bombardment of Si, Ge, and SiGe (100) surfaces* Surface Science 2016, Vol. 646, pp 253-260 (<http://dx.doi.org/10.1016/j.susc.2015.08.019>)

- Forcefield designed for bombardment of Si, Ge and SiGe surfaces with atomic hydrogen.
- Branch: combustion.

CHONSFPtCINI.ff: (C/H/O/N/S/F/Pt/Cl/Ni) Water-Pt-Ni-Nafion D.Fantauzzi, J.E. Mueller, L. Sabo, A.C.T. van Duin and T. Jacob *Surface Buckling and Subsurface Oxygen: Atomistic Insights into the Surface Oxidation of Pt(111)* ChemPhysChem, 2015, Vol.16: 2797-2802 (<http://dx.doi.org/10.1002/cphc.201500527>)

- extension of the OPt.ff forcefield parameters
- Branch: water.

CHONSSiPtZrNiCuCoHeNeArKrXe.ff: (C/H/O/N/S/Si/Pt/Zr/Ni/Cu/Co/He/Ne/Ar/Kr/Xe) A.M. Kamat, A.C.T. van Duin and A. Yakovlev *Molecular Dynamics Simulations of Laser-Induced Incandescence of Soot Using an Extended ReaxFF Reactive Force Field* *J. Phys. Chem. A*, 2010, 114 (48), pp 12561-12572 (<http://dx.doi.org/10.1021/jp1080302>)

- forcefield designed for the study of Laser-induced incandescence of soot
- Branch: combustion.

CHOSFCIN.ff: (C/H/O/S/F/Cl/N) M.A. Wood, A.C.T. van Duin and A. Strachan *Coupled Thermal and Electromagnetic Induced Decomposition in the Molecular Explosive alpha-HMX; A Reactive Molecular Dynamics Study* *J. Phys. Chem. A*, 2014, 118 (5), pp 885-895 (<http://dx.doi.org/10.1021/jp406248m>)

- forcefield designed for studying the combustion of the high-energy material a-HMX
- Branch: combustion.

Mue2016.ff: (C/H/O/S) Julian Mueller and Bernd Hartke *ReaxFF Reactive Force Field for Disulfide Mechanochemistry, Fitted to Multireference ab Initio Data;* *J. Chem. Theory Comput.*, 2016, xxx, xxx (<http://dx.doi.org/10.1021/acs.jctc.6b00461>)

- forcefield for studying S-S bond ruptures in mechanophores upon mechanical stress. Ambient conditions, both in gas phase and toluene solvent.
- Branch: combustion.

CBN.ff: (C/H/B/N) Sung Jin Pai, Byung Chul Yea and Sang Soo Han *Reactive force field for the improved design of liquid CBN hydrogen storage materials* *Phys. Chem. Chem. Phys.*, 2016, 18, pp 1818-1827 (<http://dx.doi.org/10.1039/C5CP05486A>)

- forcefield for studying liquid CBN (carbon-boron-nitrogen) hydrogen-storage materials.
- Branch: combustion.

AgZnO.ff: (C/H/O/N/Si/Cu/Ag/Zn) A.Lloyd, D. Cornil, A.C.T. van Duin, D. van Duin, R. Smith, S.D. Kenny, J. Cornil and D. Beljonne *Development of a ReaxFF potential for Ag/Zn/O and application to Ag deposition on ZnO* *Surface Science*, 2016, 645, pp 67-73 (<http://dx.doi.org/10.1016/j.susc.2015.11.009>)

- ReaxFF potential for Ag/Zn/O used to study Ag deposition on ZnO.
- Branch: water.

AlCHO.ff: (Al/C/H/O) Sungwook Hong and Adri C. T. van Duin *Atomistic-Scale Analysis of Carbon Coating and Its Effect on the Oxidation of Aluminum Nanoparticles by ReaxFF-Molecular Dynamics Simulations* *J. Phys. Chem. C*, 2016, 120 (17), pp 9464-9474 (<http://dx.doi.org/10.1021/acs.jpcc.6b00786>)

- ReaxFF potential for Al/C interactions. Used to investigate carbon coating and its effect on the oxidation of aluminum nanoparticles (ANPs)
- Branch: water.

CHNa.ff: (C/H/Na) E.Hjertenaes, A.Q. Nguyen and H. Koch *A ReaxFF force field for sodium intrusion in graphitic cathodes* *Phys. Chem. Chem. Phys.*, 2016, 18, pp 31431-31440 (<http://dx.doi.org/10.1039/C6CP06774C>)

- The force field is applied in hybrid grand canonical Monte Carlo-molecular dynamics (GC-MC/MD) simulations of model systems representative of sodium intrusion in graphitic carbon cathodes used in aluminium electrolysis.
- Branch: combustion.

CuBTC.ff: (C/H/O/N/S/Mg/P/Na/Cu) L.Huang, T. Badosz, K. L. Joshi, A. C. T. van Duin and K. E. Gubbins *Reactive adsorption of ammonia and ammonia/water on CuBTC metal-organic framework: A ReaxFF molecular dynamics simulation* *J. Chem. Phys.*, 2013, 138, 034102 (<http://dx.doi.org/10.1063/1.4774332>)

- The force field was used to study reactive adsorption of NH₃ on the dehydrated CuBTC metal-organic framework.
- Branch: water.

CHONSMgPNaTiClFAu.ff: (C/H/O/N/S/Mg/P/Na/Ti/Cl/F/Au) Susanna Monti, Vincenzo Carravetta, and Hans Ågren *Simulation of Gold Functionalization with Cysteine by Reactive Molecular Dynamics* *J. Phys. Chem. Lett.*, 2016, 7 (2), pp 272-276 (<http://dx.doi.org/10.1021/acs.jpcclett.5b02769>)

- The force field was designed to study gold-protein interactions in water.

HOSiAILi.ff: (H/O/Si/Al/Li) Alireza Ostadhossein, Sung-Yup Kim, Ekin D. Cubuk, Yue Qi, and Adri C. T. van Duin *Atomic Insight into the Lithium Storage and Diffusion Mechanism of SiO₂/Al₂O₃ Electrodes of Lithium Ion Batteries: ReaxFF Reactive Force Field Modeling* *J. Phys. Chem. A*, 2016, 120 (13), pp 2114-2127 (<http://dx.doi.org/10.1021/acs.jpca.5b11908>)

- Developed for studying the energetics and kinetics of lithiation, as well as Li transportation within the crystalline/amorphous silica and alumina phases.

CHARHeNeKr.ff: (C/H/Ar/He/Ne/Kr) Kichul Yoon, A. Rahnamoun, J.L. Swett, V. Iberi, D.A. Cullen, I.V. Vlas-siouk, A. Belianinov, S. Jesse, X. Sang, O.S. Ovchinnikova, A.J. Rondinone, R.R. Unocic, and A.C.T. van Duin *Atomistic-Scale Simulations of Defect Formation in Graphene under Noble Gas Ion Irradiation* *ACS Nano*, 2016, 10 (9), pp 8376-8384 (<http://dx.doi.org/10.1021/acs.nano.6b03036>)

- Developed for studying noble gas ion irradiation of graphene and the subsequent effects of annealing. Lattice defects including nanopores were generated.

CHO-radiation.ff: (C/H/O) Roger Smith, K. Jolley, C. Latham, M. Heggie, A van Duin, D. van Duin, Houzheng Wu *A ReaxFF carbon potential for radiation damage studies* *Nuclear Instruments and Methods in Physics Research Section B: Beam Interactions with Materials and Atoms*, Volume 393, 15 February 2017, Pages 49-53, (<http://dx.doi.org/10.1016/j.nimb.2016.11.007>)

- Developed forcefield reproduces the formation energies of many of the defects predicted by the ab initio calculations of energetic impacts and collision cascades in graphite.
- Forcefield reproduces the formation energies of many of the defects predicted by the ab initio calculations and the energy pathways between different defect states, which are important for investigating long term defect evolution.

HOTiPd.ff: (H/O/Ti/Pd) Rafik Addou, T.P. Senftle, N. O'Connor, M.J. Janik, A.C.T. van Duin, and M. Batzill *Influence of Hydroxyls on Pd Atom Mobility and Clustering on Rutile TiO₂(011)-2 x 1* *ACS Nano*, 2014, 8 (6), pp 6321-6333 (<http://dx.doi.org/10.1021/nn501817w>)

- Developed for MC simulations of Pd on TiO₂ surfaces.

CHONSMgPNaFBLi-e.ff: (C/H/O/N/S/Mg/P/Na/F/B/Li/El/Ho) M.Islam and A.C.T van Duin *Reductive Decomposition Reactions of Ethylene Carbonate by Explicit Electron Transfer from Lithium: An eReaxFF Molecular Dynamics Study* *J. Phys. Chem. C*, 2016, 120 (48), pp 27128-27134 (<http://dx.doi.org/10.1021/acs.jpcc.6b08688>)

- This forcefield uses the ACKS2 charge model
- This forcefield is an eReaxFF forcefield
- Developed for the study of lithium-ion batteries
- NOTE: This ff uses vpar(38) for e-reaxff taper radius instead of vpar(41) that ADF-reaxff expects. This will generate a warning but should still work.

CHOFeAlNiCuScrSiGe.ff: (C/H/O/Fe/Al/Ni/Cu/S/Cr/Si/Ge) Y.Zheng, S. Hong, G. Psfogiannakis, S. Datta, B. Rayner, A.C.T. van Duin and R. Engel-Herbert *Modeling and In-situ Probing of Surface Reactions in Atomic Layer Deposition* *ACS Appl. Mater. Interfaces*, 2017, 9 (18), pp 15848-15856 (<http://dx.doi.org/10.1021/acsami.7b01618>)

- Used for studying the ALD process of Al₂O₃ from trimethylaluminum and water on hydrogenated and oxidized Ge(100) surfaces

Water2017.ff: (H/O/X) W.Zhang, A.C.T. van Duin *Second-Generation ReaxFF Water Force Field: Improvements in the Description of Water Density and OH-Anion Diffusion* *J. Phys. Chem. B*, 2017, 121 (24), pp 6021-6032 (<http://dx.doi.org/10.1021/acs.jpcc.7b02548>)

- Better description of liquid water

HSMo.ff: (H/S/Mo) A.Ostadossein, A. Rahnamoun, Y. Wang, P. Zhao, S. Zhang, V.H. Crespi, and A.C.T. van Duin *ReaxFF Reactive Force-Field Study of Molybdenum Disulfide (MoS₂)* *J. Phys. Chem. Lett.*, 2017, 8 (3), pp 631-640 (<http://dx.doi.org/10.1021/acs.jpcc.7b02902>)

- MoS₂ training set in supporting info
- strain-stress analysis

CHON2017_weak.ff: (C/H/O/N/S/Mg/P/Na/Cu/Cl/X) Weiwei Zhang and Adri C. T. van Duin *Improvement of the ReaxFF Description for Functionalized Hydrocarbon/Water Weak Interactions in the Condensed Phase* *J. Phys. Chem. B*, 2018, 122, 4083-4092 (<http://dx.doi.org/10.1021/acs.jpcc.8b01127>)

- retraining of the protein-2013 force-field (C, H, O, and N parameters for weak interactions)
- reproduces well the density of liquid water and hydrocarbons

CaSiOH.ff: (C/H/O/Ca/Si/X) Hegoi Manzano, Roland J. M. Pellenq, Franz-Josef Ulm, Markus J Buehler, and A.C.T. van Duin *Hydration of Calcium Oxide Surface Predicted by Reactive Force Field Molecular Dynamics* *Langmuir*, 2012, 28 (9), 4187-4197 (<http://dx.doi.org/10.1021/la204338m>)

- hydration of calcium oxide surface
- fitted using density functional theory calculations on gas phase calcium-water clusters, calcium oxide bulk and surface properties, calcium hydroxide, bcc and fcc Ca, and proton transfer reactions in the presence of calcium.

CHO-2016.ff: (C/H/O) Chowdhury Ashraf and Adri C.T. van Duin* *Extension of the ReaxFF Combustion Force Field toward Syngas Combustion and Initial Oxidation Kinetics* *J. Phys. Chem. A* 121, 5, 1051-1068 (<https://dx.doi.org/10.1021/acs.jpca.6b12429>)

- improved description of oxidation of small hydrocarbons and syngas reaction

CHON2017_weak_bb.ff: (C/H/O/N/S/Mg/P/Na/Cu/Cl/X) Vashisth A., Ashraf C., Zhang W., Bakis C.E., van Duin A.C.T. *Accelerated ReaxFF Simulations for Describing the Reactive Cross-Linking of Polymers* *J Phys Chem A*. 2018 Aug 1. (<https://doi.org/10.1021/acs.jpca.8b03826>)

- reparametrized version of CHON2017_weak.ff for bond-boost application

CH_aromatics.ff: (C/H) Qian Mao, Yihua Ren, K. H. Luo, Adri C. T. van Duin *Dynamics and kinetics of reversible homo-molecular dimerization of polycyclic aromatic hydrocarbons* *The Journal of Chemical Physics* 147, 244305 (2017) (<https://doi.org/10.1063/1.5000534>)

- ff for polycyclic aromatic hydrocarbons

CuSCH.ff: (C/H/O/S/Cu/Cl/X) Jejoon Yeon, Heather L. Adams, Chad E. Junkermeier, Adri C. T. van Duin, Wilfred T. Tysoe, and Ashlie Martini *Development of a ReaxFF Force Field for Cu/S/C/H and Reactive MD Simulations of Methyl Thiolate Decomposition on Cu (100)* *J. Phys. Chem. B*, 2018, 122 (2), pp 888-896 (<https://doi.org/10.1021/acs.jpcc.7b06976>)

- combination of CuCl-H₂O.ff and AuSCH_2011.ff
- reparametrized Cu-S parameters with copper sulfides data

TiO₂bio.ff: (C/H/O/N/S/Mg/P/Na/Ti/Cl/F/X) Susanna Monti, Mariachiara Pastore, Cui Li, Filippo De Angelis, and Vincenzo Carravetta *Theoretical Investigation of Adsorption, Dynamics, Self-Aggregation, and Spectroscopic*

Properties of the D102 Indoline Dye on an Anatase (101) Substrate J. Phys. Chem. C, 2016, 120 (5), pp 2787-2796 (<https://doi.org/10.1021/acs.jpcc.5b11332>)

CHFe.ff: (C/H/Fe) Md Mahbulul Islam, Chenyu Zou, Adri C. T. van Duin and Sumathy Raman *Interactions of hydrogen with the iron and iron carbide interfaces: a ReaxFF molecular dynamics study* Phys. Chem. Chem. Phys., 2016, 18, 761-771 (<https://doi.org/10.1039/C5CP06108C>)

FORCE FIELD FORMAT SPECIFICATION

Each force field file consist of following sections:

| Section name | N of params | N of header lines | N of block keys | block keys |
|----------------|-------------|-------------------|-----------------|-----------------|
| General | 41 | 1 | | |
| Atoms | 32 | 4 | 1 | atom type name |
| Bonds | 16 | 2 | 2 | atom type index |
| Off-diagonal | 6 | 1 | 2 | atom type index |
| Angles | 7 | 1 | 3 | atom type index |
| Torsions | 7 | 1 | 4 | atom type index |
| Hydrogen bonds | 4 | 1 | 2 | atom type index |

9.1 Format

The force field file begins with a description line that, in turn, may optionally begin with a list of keywords between square brackets, for example (for an ACKS2+eReaxff force-field):

```
[ ereaxff acks2 ] Reactive MD-force field for Ethylene Carbonate and Li
```

Each section starts with one or more header line containing, on the first line, the number of blocks in the section, possibly followed by description of the parameters. The number of header lines is supposed to match the number lines in a block of the corresponding section (4 in atoms, 2 in bonds and 1 in every other section). The additional header lines after the first are skipped when reading the force field file.

General parameters

The header of this section starts with *npar*, the number of general parameters present in the force field file. The header is followed by *npar* lines each containing a parameter value followed by a comment, for example:

```
39      ! Number of general parameters
50.0000 !Overcoordination parameter
```

Atoms

The atomic parameters section starts with the number of atom types present in the force field, followed by three additional header lines and the blocks of parameters, one block per atom type. Each block consists of 4 lines starting with a line containing the atom name and 8 parameter values with the (1x,a2,8f9.4) format followed by three lines with 8 parameter values each, with the (3x,8f9.4) format, for example:

```
3      ! Nr of atoms; cov.r; valency;a.m;Rvdw;Evdw;gammaEEM;cov.r2;#
      alfa;gammavdW;valency;Eunder;Eover;chiEEM;etaEEM;n.u.
```

(continues on next page)

(continued from previous page)

```

cov r3;Elp;Heat inc.;n.u.;n.u.;n.u.;n.u.
ov/un;vall;n.u.;val3,vval4
C  1.3817  4.0000  12.0000  1.8903  0.1838  0.  9000  1.1341  4.0000
   9.7559  2.1346  4.0000  34.9350  79.5548  5.  9666  7.0000  0.0000
   1.2114  0.0000 202.5551  8.9539  34.9289 13.  5366  0.8563  0.0000
  -2.8983  2.5000  1.0564  4.0000  2.9663  0.  0000  0.0000  0.0000
H   0.7853  1.0000  1.0080  1.5904  0.0419  1.0206 -0.1000  1.0000
   9.3557  5.0518  1.0000  0.0000 121.1250  5.3200  7.4366  1.0000
  -0.1000  0.0000  62.4879  1.9771  3.3517  0.7571  1.0698  0.0000
 -15.7683  2.1488  1.0338  1.0000  2.8793  0.0000  0.0000  0.0000
... one more block ...

```

Bonds, angles, etc.

In the remaining sections, a block key consists of two or more integer numbers, each of them referring to the atomic block with this index. The number of integers in the key depends on the block type (two for bonds, three for valence angles, etc.). For instance, the bond parameters block below corresponds to the C-H bond for the atoms block shown above.

The bond parameters section starts with the number of bond types followed by one additional comment line. The first line of the block has the (2i3,8f9.4) format and the second (6x,8f9.4):

```

6      ! Nr of bonds; Edis1; Lppen;n.u.;pbe1;pbo5;l3corr;pbo6
      pbe2;pbo3;pbo4;n.u.;pbo1;pbo2;ovc  orr
1  1 156.5953 100.0397  80.0000 -0.8157 -0.4591  1.0000  37.7369  0.4235
      0.4527 -0.1000  9.2605  1.0000 -0.0750  6.8316  1.0000  0.0000
... five more blocks ...

```

For the rest of the sections, the format remains similar to the bonds section, except that they do not have additional header lines and the Fortran format may be slightly different: (2i3,6f9.4) for off-diagonal, (3i3,7f9.4) for valence angles, (4i3,7f9.4) for torsion angles, and (3i3,4f9.4) for hydrogen bonds.

9.2 Equation Reference

In the tables below the ReaxFF parameters are listed with their corresponding equation numbers from the SCM developer notes which have mostly technical relevance. For a good introduction to the meaning of ReaxFF parameters we advise the initial ReaxFF publication [ReaxFF: A Reactive Force Field for Hydrocarbons](https://doi.org/10.1021/jp004368u), A.C.T. van Duin, S. Dasgupta, F. Lorant, W.A. Goddard, J. Phys. Chem. A. 2001 105 41 9396-9409. (<https://doi.org/10.1021/jp004368u>)

General

Of particular interest are the upper taper radius parameter (#13), which describes the non-bonded cutoff radius, and the bond order cutoff (#30), which describes the bond order threshold, above which atoms are considered connected. Both these parameters may have a major impact on the ReaxFF calculation speed; decreasing the taper radius or increasing the bond order cutoff can make ReaxFF run considerably faster. These parameters, however, have a significant impact on the force description and should not be changed without re-parameterization of other parts of the force field.

| Index | Name in Eq | Equation | Comment |
|-------|------------|----------|-------------------------------------|
| 1 | p_boc1 | 4c | Overcoordination parameter |
| 2 | p_boc2 | 4d | Overcoordination parameter |
| 3 | -p_coa2 | 15 | Valency angle conjugation parameter |
| 4 | p_trip4 | 20 | Triple bond stabilization parameter |
| 5 | p_trip3 | 20 | Triple bond stabilization parameter |

Continued on next page

Table 9.1 – continued from previous page

| | | | |
|----|--------------|---------------|---|
| 6 | k_c2 | 19 | C2-correction |
| 7 | p_ovun6 | 12 | Undercoordination parameter |
| 8 | p_trip2 | 20 | Triple bond stabilization parameter |
| 9 | p_ovun7 | 12 | Undercoordination parameter |
| 10 | p_ovun8 | 12 | Undercoordination parameter |
| 11 | p_trip1 | 20 | Triple bond stabilization energy |
| 12 | n/a | 21 | Lower Taper-radius |
| 13 | R_cut | 21 | Upper Taper-radius |
| 14 | p_fe1 | 6a | Fe dimer correction |
| 15 | p_val6 | 13c | Valency undercoordination |
| 16 | p_lp1 | 8 | Valency angle/lone pair parameter |
| 17 | p_val9 | 13f | Valency angle parameter |
| 18 | p_val10 | 13g | Valency angle parameter |
| 19 | p_fe2 | 6a | Fe dimer correction |
| 20 | p_pen2 | 14a | Double bond/angle parameter |
| 21 | p_pen3 | 14b | Double bond/angle parameter: overcoord |
| 22 | p_pen4 | 14b | Double bond/angle parameter: overcoord |
| 23 | p_fe3 | 6a | Fe dimer correction |
| 24 | p_tor2 | 16b | Torsion/BO parameter |
| 25 | p_tor3 | 16c | Torsion overcoordination |
| 26 | p_tor4 | 16c | Torsion overcoordination |
| 27 | p_elho | 26a | eReaxFF |
| 28 | p_cot2 | 17b | Conjugation |
| 29 | p_vdW1 | 23b | VdW shielding |
| 30 | cutoff * 100 | 3a,b | Cutoff for bond order (* 100) |
| 31 | p_coa4 | 15 | Valency angle conjugation parameter |
| 32 | p_ovun4 | 11b | Overcoordination parameter |
| 33 | p_ovun3 | 11b | Overcoordination parameter |
| 34 | p_val8 | 13d | Valency/lone pair parameter |
| 35 | X_soft | 25 | ACKS2 softness parameter |
| 36 | unused | n/a | n/a |
| 37 | p_val | 27 via n_el | eReaxFF |
| 38 | n/a | 13d | if 1: remove delta_j term for non-C-C-C angles and where none of the atoms is N |
| 39 | p_coa3 | 15 | Valency angle conjugation parameter |
| 40 | n/a | 20 | Condition to turn triple bond option: vpar(40) == 1 |
| 41 | n/a | 26 via Tap(R) | eReax-specific taper radius for interactions with/between electrons and holes |

Atoms

If negative values are provided to either of the three bond radii (**sigma**, **pi**, and **double pi**) the bond order contributions are ignored for that atom.

| Index | Name in Eq | Equation | Comment |
|-------|------------|---------------|-----------------------------------|
| 1 | r_0^sigma | 2 | Sigma bond covalent radius |
| 2 | Val_i | 3a, 4b, 5, 9a | Valency |
| 3 | n/a | 9a | Atomic mass |
| 4 | r_vdW | 23a | van der Waals radius |
| 5 | D_ij | 23a | van der Waals dissociation energy |

Continued on next page

Table 9.2 – continued from previous page

| | | | |
|----|----------------|------------|---|
| 6 | gamma_i | 24 | gammaEEM; EEM shielding |
| 7 | r_0^pi | 2 | Pi bond covalent radius |
| 8 | Val_i^e | 7, 8, 9 | Number of valence electrons |
| 9 | alpha_ij | 23b | van der Waals parameter |
| 10 | 1/gamma_w | 23b | van der Waals shielding |
| 11 | Val_j^angle | 16c, 13c | Valency for 1,3-BO correction |
| 12 | p_ovun5 | 12 | Undercoordination energy |
| 13 | p_i^xel2 | 26 | eReaxFF, atom type parameter |
| 14 | chi_i | 24, 25 | EEM electronegativity |
| 15 | eta_i | 24, 25 | EEM hardness |
| 16 | n/a | n/a | Donor or acceptor switch in H-bonds |
| 17 | r_0^pi | 2 | Double pi bond covalent radius |
| 18 | p_lp2 | 10 | Lone pair energy |
| 19 | n/a | n/a | Atomic heat of formation |
| 20 | p_boc4 | 4e,f | Bond order correction |
| 21 | p_boc3 | 4e,f | Bond order correction |
| 22 | p_boc5 | 4e,f | Bond order correction |
| 23 | C_i | 25 | Atomic softness cutoff parameter |
| 24 | alpha, alpha_i | 26, 26a | eReaxFF, constant, dependent on atom type |
| 25 | p_ovun2 | 12 | Valence angle parameter |
| 26 | p_val3 | 13b -> 13a | Valence angle parameter |
| 27 | beta, beta_i | 26a | eReaxFF, constant, dependent on atom type |
| 28 | Val_i'^boc | 3b | Number of lone pairs |
| 29 | p_val5 | 13b | Valence angle parameter |
| 30 | p_c1 | 23c | Inner wall vdW repulsion parameter |
| 31 | p_c2 | 23c | Inner wall vdW repulsion parameter |
| 32 | p_c3 | 23c | Inner wall vdW repulsion parameter |
| 33 | C_i | 23d | Lg dispersion parameter |
| 34 | R_eij | 23d | VdW Radius for Lg dispersion correction |

Bonds

| | | | |
|----|------------|--------|--|
| 1 | D_e^sigma | 6, 11a | Sigma-bond dissociation energy |
| 2 | D_e^pi | 6 | Pi-bond dissociation energy |
| 3 | D_e^pipi | 6 | Double pi-bond dissociation energy |
| 4 | p_be1 | 6 | Bond energy parameter |
| 5 | p_bo5 | 2 | Double pi bond parameter |
| 6 | Val'_i^boc | 3b | 1,3-Bond order correction |
| 7 | p_bo6 | 2 | Double pi bond order |
| 8 | p_ovun1 | 11a | Overcoordination penalty |
| 9 | p_be2 | 6 | Bond energy parameter |
| 10 | p_bo3 | 2 | Pi bond order parameter |
| 11 | p_bo4 | 2 | Pi bond order parameter |
| 12 | unused | n/a | n/a |
| 13 | p_bo1 | 2 | Sigma bond order |
| 14 | p_bo2 | 2 | Sigma bond order |
| 15 | delta'_i | 3a | Uncorrected BO overcoordination |
| 16 | p_ij^xel1 | 27 | e ReaxFF param; for adjusting number of electrons available to host atom |

Off-diagonal

This section allows for the definition of off-diagonal values for both bond order and van der Waals pair interactions. By default, ReaxFF calculates these terms from the combination rules and the atom parameters (i.e. the default C-H van der Waals radius is $(R_{vdW}[C]*R_{vdW}[H])^{0.5}$), but the off-diagonal section allows for the definition of different values. Any value given in the off-diagonal section overrules that obtained from the combination rules.

| | | | |
|---|--------------|-----|-------------------------|
| 1 | D_ij | 23a | VdW energy |
| 2 | r_vdW | 23a | VdW radius |
| 3 | alpha_ij | 23a | VdW parameter |
| 4 | r_0^sigma | 2 | Sigma bond length |
| 5 | r_0^pi | 2 | Pi bond length |
| 6 | r_0^pipi | 2 | PiPi bond length |
| 7 | C_i, C_lg,ij | 23d | Lg dispersion parameter |

Angles

| | | | |
|---|-----------|------------|--------------------------|
| 1 | Theta_0,0 | 13g | 180o-(equilibrium angle) |
| 2 | p_val1 | 13a | Valence angle parameter |
| 3 | p_val2 | 13a | Valence angle parameter |
| 4 | p_coa1 | 15 | Valence conjugation |
| 5 | p_val7 | 13c | Undercoordination |
| 6 | p_pen1 | 14b -> 14a | Penalty energy |
| 7 | p_val4 | 13b | Valence angle parameter |

Torsions

| | | | |
|---|--------|-----|-------------------------|
| 1 | V_1 | 16a | V1-torsion barrier |
| 2 | V_2 | 16a | V2-torsion barrier |
| 3 | V_3 | 16a | V3-torsion barrier |
| 4 | p_tor1 | 16a | Torsion angle parameter |
| 5 | p_cot1 | 17a | Conjugation energy |
| 6 | unused | n/a | n/a |
| 7 | unused | n/a | n/a |

Hydrogen bonds

| | | | |
|---|--------|----|------------------------------------|
| 1 | r_hb^0 | 18 | Hydrogen bond equilibrium distance |
| 2 | p_hb1 | 18 | Hydrogen bond energy |
| 3 | -p_hb2 | 18 | Hydrogen bond/bond order |
| 4 | -p_hb3 | 18 | Hydrogen bond parameter |

TROUBLESHOOTING AND WARNINGS

10.1 Geometry optimization issues

Geometry optimization issues with ReaxFF are usually caused by the fact that the derivative of the ReaxFF energy function has discontinuities. These discontinuities are often related to the bond order cutoff (the `Engine ReaxFF%BondOrderCutoff` key, 0.001 by default). This cutoff determines whether a valence or a torsion angle is included in the potential energy evaluation or not, i.e. when at least one of the bonds forming an angle is of order lower than the cutoff then the angle is discarded. Thus, when the order of a particular bond crosses the cutoff value between two optimization steps, the energy derivative (the force) experiences a sudden change. The magnitude of the jump depends on the cutoff value. The default value of 0.001 is normally not a problem during molecular dynamics but it may break the geometry optimization convergence.

There are a several ways to reduce the discontinuity and thus to improve the stability of the geometry optimization.

- **Use 2013 torsion angles (set `Engine ReaxFF%Torsions` to 2013):** Switch on the 2013 formula for the torsion angles. This will make the torsion angles change more smoothly at lower bond orders but it will not affect the valence angles. You should be aware, however, that using this option changes the bond order dependence of the ReaxFF 4-center term.
- **Decrease the bond order cutoff (`Engine ReaxFF%BondOrderCutoff`):** This will significantly reduce the discontinuity in the valence angles and somewhat in the torsion angles but will not remove it. This will also make the calculation somewhat slower because more angles will have to be included in the computation.
- **Taper the bond orders (`Engine ReaxFF%TaperBO`):** Use tapered bond orders by Furman and Wales (DOI: 10.1021/acs.jpcclett.9b02810).

10.2 Warnings

WARNING: Inconsistent vdWaals-parameters in forcefield. See output All atom types in a force-field file should normally have consistent Van der Waals screening and short-range repulsion (a.k.a. inner core) parameters. This warning is printed if two atom types have inconsistent parameters.

WARNING: Suspicious force-field EEM parameters for ... For every atom type, the eta and gamma parameters for the electronegativity equalization method (EEM) should satisfy the relation: $\eta > 7.2 \cdot \gamma$. Otherwise a polarization catastrophe is likely to occur at a short interatomic distance, the critical distance being dependent on the eta/gamma ratio. The smaller the ratio the larger the distance at which this occurs. When the polarisation catastrophe occurs the amount of charge that flows from one atom to the other can become very large. The EEM routine checks that the resulting charge for each atom lies within the $[-10, Z]$ interval, where Z is the number of electrons in the neutral atom, and throws an error if the check fails.

REQUIRED CITATIONS

When you publish results in the scientific literature that were obtained with programs of the ADF package, you are required to include references to the program package with the appropriate release number, and a few key publications.

In addition to these general references, references to special features are mandatory, in case you have used them.

11.1 General References

The ReaxFF software that SCM makes available is based on the ReaxFF program developed by Adri van Duin.

For calculations with ReaxFF:

1. A.C.T. van Duin, S. Dasgupta, F. Lorant, and W. A. Goddard, *ReaxFF: A reactive force field for hydrocarbons*, *Journal of Physical Chemistry A* 105, 9396-9409 (2001) (<https://doi.org/10.1021/jp004368u>)
2. K. Chenoweth, A.C.T. van Duin, and W.A. Goddard, *ReaxFF reactive force field for molecular dynamics simulations of hydrocarbon oxidation*, *Journal of Physical Chemistry A* 112, 1040-1053 (2008) (<https://doi.org/10.1021/jp709896w>)
3. ReaxFF 2020, SCM, Theoretical Chemistry, Vrije Universiteit, Amsterdam, The Netherlands, <http://www.scm.com> Optionally, you may add the following list of authors and contributors: A.C.T. van Duin, W.A. Goddard, M.M. Islam, H. van Schoot, T. Trnka, A.L. Yakovlev

The ReaxFF GUI (ReaxFFinput and AMSmovie) has been developed within SCM (with O. Visser as primary developer).

The ReaxFF program has been parallelized, optimized, and extended by SCM (with A.L. Yakovlev as primary developer).

If you use one of the included force fields you must also add the *proper reference for it* (page 17).

Many examples of ReaxFF applications can be found on Prof. van Duin's publication list (<http://www.engr.psu.edu/adri/Publications.aspx>).

11.2 Feature References

When you have used force fields or special features, you should include the reference(s) to the implementation.

Collective Variable-Driven Hyperdynamics (CVHD) K.M. Bal and E.C. Neyts, *Merging Metadynamics into Hyperdynamics: Accelerated Molecular Simulations Reaching Time Scales from Microseconds to Seconds*, *J. Chem. Theory Comput.*, 11, 4545-4554 (2015) (<https://doi.org/10.1021/acs.jctc.5b00597>)

Force-bias Monte Carlo (fbMC) M.J. Mees, G. Pourtois, E.C. Neyts, B.J. Thijsse, A. Stesmans, *Uniform-acceptance force-bias Monte Carlo method with time scale to study solid-state diffusion*, *Physical Review B* **85**, 134301 (2012) (<https://doi.org/10.1103/PhysRevB.85.134301>)

Grand Canonical Monte Carlo (GCMC) Th.P. Senftle, R.J. Meyer, M.J. Janik and A.C.T. van Duin, *Development of a ReaxFF potential for Pd/O and application to palladium oxide formation*, *J. Chem. Phys.* **139**, 044109 (2013) (<https://doi.org/10.1063/1.4815820>)

Th.P. Senftle, A.C.T. van Duin, M.J. Janik, *Determining in situ phases of a nanoparticle catalyst via grand canonical Monte Carlo simulations with the ReaxFF potential*, *Catalysis Communications* ****volume 52****, 5 July 2014, Pages 72–77 (<https://doi.org/10.1016/j.catcom.2013.12.001>)

Monte-Carlo force-field optimizer (MCFFOptimizer)

E. Iype, M. Huetter, A.P.J. Jansen, S.V. Nedeia, C.C.M. Rindt, *Parameterization of a Reactive Force Field Using a Monte Carlo Algorithm*, *J. Comp. Chem.* **34**, 1143-1154 (2013) (<https://doi.org/10.1002/jcc.23246>)

ACKS2

T. Verstraelen, P.W. Ayers, V. Van Speybroeck, M. Waroquier, *ACKS2: Atom-Condensed Kohn-Sham DFT Approximated to Second Order* *J. Chem. Phys.* **138**, 074108 (2013) (<https://doi.org/10.1063/1.4791569>)

eReaxFF M.M. Islam, G. Kolesov, T. Verstraelen, E. Kaxiras, A.C.T. van Duin, *eReaxFF: A Pseudoclassical Treatment of Explicit Electrons within Reactive Force Field Simulations*, *J. Chem.Theory Comput* **12**, 3463 (2016) (<https://doi.org/10.1021/acs.jctc.6b00432>)

ReaxFF Force Field References When you publish results in the scientific literature that were obtained with one of the included force fields for ReaxFF, including the proper reference for the force field used is mandatory.

- *Forcefields included in the latest release* (page 17)
- *Forcefields included in the development snapshots* (page 31)

Reaction Event Detection (ChemTraYzer) M. Döntgen, M.-D. Przybylski-Freund, L.C. Kröger, W.A. Kopp, A.E. Ismail, K. Leonhard *Automated Discovery of Reaction Pathways, Rate Constants, and Transition States Using Reactive Molecular Dynamics Simulations* (<https://doi.org/10.1021/acs.jctc.5b00201>) *J. Chem.Theory Comput.*, **11** (6), 2517–2524, 2015

11.3 External programs and Libraries

[Click here](#) for the list of programs and/or libraries used in the ADF package. On some platforms optimized libraries have been used and/or vendor specific MPI implementations.

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