ReaxFF Manual

Amsterdam Modeling Suite 2026.1

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CONTENTS

CHAPTER

ONE

GENERAL

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 11) 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 15).

Other new features:

- 0D, 1D, and 2D periodicity
- *Tapered bond orders* (page 4)
- *Charge constraints* (page 8)

Note: Development of the old standalone ReaxFF program (https://www.scm.com/doc.2024/OldReaxFF/index.html) has stopped.

CHAPTER TWO

REAXFF INPUT

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

See also:

- *AMS driver's tasks and properties* (page 11)

2.1 Force field specification

The only input key required by the engine is `ForceField`, used to select the *force field file* (page 43). Force fields *included in the Amsterdam Modeling Suite* (page 21) can be easily accessed using their file name, such as `CHO.ff`.

`ForceField`

Type
String

Description
Path to the force field parameter file. The path can be absolute or relative. Relative paths starting with ./ are considered relative to the directory in which the calculation is started, otherwise they are considered relative to $AMSRESOURCES/ForceFields/ReaxFF.

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.jpclett.9b02810).

`TaperBO`

Type
Bool

Default value
No

GUI name
Taper bond orders

Description
Use tapered bond orders by Furman & Wales (DOI: 10.1021/acs.jpclett.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). The new expression for each term in f_{10} is $\left(1 - e^{-2\lambda_{23}\mathrm{BO}^2}\right)$ and in f_{12} the new expression is $\sin(\frac{\pi}{3}\mathrm{BO})^4$. The new expressions ensure correct asymptotic behavior for the $\frac{dE}{d\mathrm{BO}}$ for $\mathrm{BO} \to 0$.

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 49)

`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 3- and 4-body potentials.

`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]
   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
```

Sometimes it may be useful to disable the charge equilibration altogether and set the charges from input. This can be done using the `reaxff.charge` atom property, as shown in the example below:

```
System
    Atoms
        O -0.0509 -0.2754  0.6371 reaxff.charge=-0.8
        H  0.0157  0.5063  0.0531 reaxff.charge=0.4
        H -0.0055 -1.0411  0.0658 reaxff.charge=0.4
        O  0.0981  1.7960 -1.2550 reaxff.charge=-0.8
        H -0.6686  2.2908 -1.5343 reaxff.charge=0.4
        H  0.8128  2.3488 -1.5619 reaxff.charge=0.4
    End
End
```

2.7 Atomic stress (per-atom stress tensor)

The per-atom stress tensor is calculated according to Thompson, Plimpton, Mattson, J Chem Phys, 131, 154107 (2009) (https://doi.org/10.1063/1.3245303) . It does not include any kinetic contribution (i.e., it is atomic stress, not atomic pressure).

The calculated stress tensor is stored in the engine .rkf file in the `RxfAtomData%AtomicStressIso` variable in MPa. It is calculated as $S\alpha\beta/V$, where V is atomic volume calculated using the Voronoi partitioning scheme.

`ComputeAtomicPressure`

Type
Bool

Default value
No

Description
Compute the virial part of the atomic pressure (the kinetic part cannot be computed by the engine).

CHAPTER

THREE

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

CHAPTER
FOUR

EREAXFF, ACKS2, LG DISPERSION

Note: Only the *ReaxFF force fields* (page 21) 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 explicitly[1].

An eReaxFF calculation **requires the following additional force-field parameters to be defined** (equation numbers are referring to the eReaxFF paper[1]):

- 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 14), the ACKS2-related parameters should also be defined.

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

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

---

[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

4.2 ACKS2 charge equilibration

The ACKS2 charge equilibration scheme has been implemented following the original paper[2].

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.

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[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

[3] L. Liu at 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

CHAPTER

FIVE

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 (https://www.scm.com/doc.2024/OldReaxFF/index.html)

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	*force field file* (page 14)	old manual entry (https://www.scm.com/doc.2024/OldReaxFF/Miscellaneous.html#acks2-atom-condensed-kohn-sham-dft-approximated-to-second-order)
Adsorption analysis	AMS driver	old manual entry (https://www.scm.com/doc.2024/OldReaxFF/Properties.html#adsorption-analysis)
Bond boost	AMS driver	old manual entry (https://www.scm.com/doc.2024/OldReaxFF/BondBoost.html)
ChemTraYzer	AMS utilities	old manual entry (https://www.scm.com/doc.2024/OldReaxFF/ChemTraYzer.html)
CMAES FF optimizer	ParAMS	old manual entry (https://www.scm.com/doc.2024/OldReaxFF/CMAESFFOptimizer.html)
CVHD	AMS driver	old manual entry (https://www.scm.com/doc.2024/OldReaxFF/CVHD.html)
Elastic wall restraint	not available	old manual entry (https://www.scm.com/doc.2024/OldReaxFF/Miscellaneous.html#elastic-wall-restraint)
eReaxFF	*force field file* (page 13)	old manual entry (https://www.scm.com/doc.2024/OldReaxFF/eReaxFF.html)
External electric fields	AMS driver	old manual entry (https://www.scm.com/doc.2024/OldReaxFF/Miscellaneous.html#external-electric-fields)
Force-bias Monte Carlo	AMS driver	old manual entry (https://www.scm.com/doc.2024/OldReaxFF/fbMC.html)
Force field parametrization	ParAMS	old manual entry (https://www.scm.com/doc.2024/OldReaxFF/FFOptimizer.html)
Grand-canonical Monte Carlo	AMS driver	old manual entry (https://www.scm.com/doc.2024/OldReaxFF/GCMC.html)
Local atomic temperature	not available	old manual entry (https://www.scm.com/doc.2024/OldReaxFF/Properties.html#local-atomic-temperature)
LG dispersion	*force field file* (page 14)	old manual entry (https://www.scm.com/doc.2024/OldReaxFF/Miscellaneous.html#lg-dispersion)
Molecular charge constraints	*ReaxFF Engine* (page 8)	old manual entry (https://www.scm.com/doc.2024/OldReaxFF/Miscellaneous.html#molecular-charges)
Molecule gun	AMS driver	old manual entry (https://www.scm.com/doc.2024/OldReaxFF/molgun.html)
NEMD (thermal conductivity)	AMS driver	old manual entry (https://www.scm.com/doc.2024/OldReaxFF/Properties.html#nemd-methods-for-thermal-conductivity)
Per-atom stress tensor	*ReaxFF engine* (page 9)	old manual entry (https://www.scm.com/doc.2024/OldReaxFF/Properties.html#atomicstresstensor)
Tapered bond orders	*ReaxFF engine* (page 4)	old manual entry (https://www.scm.com/doc.2024/OldReaxFF/Miscellaneous.html#correction-for-small-bond-orders)
Temperature profile along axis	AMS driver	old manual entry (https://www.scm.com/doc.2024/OldReaxFF/Properties.html#temperature-profile-along-coordinate-axis)
Volume regimes	AMS driver	vregime.in Training Course (https://www.scm.com/doc.2024/OldReaxFF/index.html#other-reax-ff-manuals)

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 (https://www.scm.com/doc.2024/OldReaxFF/index.html).

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

CHAPTER

SIX

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 methods 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.

CHAPTER

SEVEN

INCLUDED FORCE FIELDS

Disclaimer: These force fields have been trained for specific systems, details of which are provided in the accompanying manuscripts (and briefly summarized below). Using the forcefields for systems outside the scope of the training data may produce unrealistic results.

Note: Try out AMS-ReaxFF with a free trial (https://www.scm.com/free-trial/) and explore the ReaxFF Tutorials. When you build your system, the GUI only displays ReaxFF force fields including bonded parameters for your combination of elements. You can create new ReaxFF force fields or reparametrize existing ones with ParAMS.

The force field files used by the SCM version of ReaxFF are compatible with those used by the original ReaxFF code. Force fields obtained from external sources are useable as long as they use the standard ReaxFF format. (You can select them in AMSinput using the `Other...` option).

There are currently two major 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, 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 (https://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 (https://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*, J. Mat. Chem. 2010, 20, 10431-10437 (https://dx.doi.org/10.1039/C0JM01556C)

  - Au/C/S/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. C, 2011, 115, 10315-10322 (https://dx.doi.org/10.1021/jp201496x)
  - C/O/H/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*, J. Phys. Chem. B, 2011, 115, 249-261 (https://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, and W. A. Goddard III, *ReaxFF Reactive Force Field for Molecular Dynamics Simulations of Hydrocarbon Oxidation*, J. Phys. Chem. A, 2008, 112, 1040-1053 (https://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 (https://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*, J. Phys. Chem. A, 2010, 114, 12561-1257 (https://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 (https://dx.doi.org/10.1016/j.combustflame.2011.10.022)
- The C/H/O parameters are the same as in the CHO.ff forcefield, with added S/C, S/H and S/O descriptions from Castro-Marcano et al.
- The Boron and Nitrogen parameters are based on (but not identical to) the parameters used by Weismiller et al.
- 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, 2010, 114, 3556-3568 (https://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 (https://dx.doi.org/10.1021/jp102272z)
- Branch: water.

FeOCHCl.ff: (Fe/O/C/H/Cl)

M. Aryanpour, A.C.T. van Duin, and J.D. Kubicki, *Development of a Reactive Force Field for Iron-Oxyhydroxide Systems*, J. Phys. Chem. A, 2010, 114, 6298-6307 (https://dx.doi.org/10.1021/jp101332k)

- The Cl parameters where 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, 2010, 114, 3556-3568 (https://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.

FeOCHCl-ox.ff: (Fe/O/C/H/Cl)

M. Aryanpour, A.C.T. van Duin, and J.D. Kubicki, *Development of a Reactive Force Field for Iron-Oxyhydroxide Systems*, J. Phys. Chem. A, 2010, 114, 6298-6307 (https://dx.doi.org/10.1021/jp101332k)

- Compared to FeOCHCl.ff, Fe/O/H parameters have been reparametrized using iron oxide bulk data.
- Detailed information on the force field parameters is given in the supporting information of the corresponding 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 III, *Thermal Decomposition of Hydrazines from Reactive Dynamics Using the ReaxFF Reactive Force Field*, J. Phys. Chem. B, 2009, 113, 10770-10778 (https://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 III, 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*, J. Phys. Chem. A, 2009, 113, 10619-10640 (https://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 (https://dx.doi.org/10.1103/PhysRevLett.91.098301) for a detailed description of the parametrization 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 III, 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*, J. Phys. Chem. A, 2009, 113, 10619-10640 (https://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 III, *Modeling the sorption dynamics of NaH using a reactive force field*, J. Chem. Phys. 2008, 128, 164714 (https://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 (https://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, and S.A. Pandit, *A reactive molecular dynamics simulation of the silica-water interface*, J. Chem. Phys. 2010, 132, 174704 (https://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*, J. Phys. Chem. C, 2012, 116, 16111-16121 (https://dx.doi.org/10.1021/jp306391p)

- The included forcefield is based on the original Newsome publication, with slightly improved parameters contributed by A.C.T. van Duin.
- Branch: combustion.

VOCH.ff: (V/O/C/H)

K. Chenoweth, A.C.T. van Duin, P. Persson, M.J. Cheng, J. Oxgaard, and W.A. Goddard III, *Development and Application of a ReaxFF Reactive Force Field for Oxidative Dehydrogenation on Vanadium Oxide Catalysts*, J. Phys. Chem. C, 2008, 112, 14645-14654 (https://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, and K. Hermannson, *A reactive force field (ReaxFF) for zinc oxide*, Surf. Sci. 2008, 602, 1020-1031 (https://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 III, and K. Hermansson, *Water adsorption on stepped ZnO surfaces from MD simulation*, Surf. Sci. 2010, 604, 741-752 (https://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*, Int. J. Hydrog. Energy, 2011, 36, 5828-5835 (https://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, 3042-3053 (https://dx.doi.org/10.1021/ja208894m)

- Branch: water.

dispersion/CHONSSi-lg.ff: (C/H/O/N/S/Si)
L. Liu, Y. Liu, S.V. Zybin, H. Sun, and W.A. Goddard III, *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, 11016-11022 (https://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*, J. Phys. Chem. B, 2011, 115, 249-261 (https://dx.doi.org/10.1021/jp204894m)

- 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, 12163-12174 (https://dx.doi.org/10.1021/jp308507x)
- Not all crossterms 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, 2011, 115, 10315-10322 (https://dx.doi.org/10.1021/jp201496x)

- Branch: combustion.

AuSCH_2013.ff: (Au/S/C/H)
G.T. Bae and C.M. Aikens, *Improved ReaxFF Force Field Parameters for Au-S-C-H Systems*, J. Phys. Chem. A, 2013, 117, 10438-10446 (https://dx.doi.org/10.1021/jp405992m)

- Based upon: 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. C, 2011, 115, 10315-10322 (https://dx.doi.org/10.1021/jp201496x)
- 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, 7192-7202 (https://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*, J. Mat. Research, 2013, 28, 513-520 (https://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, 2008, 112, 1392-1402 (https://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, 2008, 112, 3133-3140 (https://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, 2005, 109, 493-499 (https://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, 2011, 115, 249-261 (https://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, 258-269 (https://dx.doi.org/10.1021/jp3086649)

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

CHOFe.ff: (C/H/O/Fe/Cl/Si/Al)

Chenyu Zou and A.C.T. Van Duin, *Investigation of Complex Iron Surface Catalytic Chemistry Using the ReaxFF Reactive Force Field Method*, JOM, 2012, 64, 1426-1437 (https://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-Marcanoa and A.C.T. van Duin, *Comparison of thermal and catalytic cracking of 1-heptene from ReaxFF reactive molecular dynamics simulations*, Combustion and Flame, 2013, 160, 766-775 (https://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, and A.C.T. van Duin *Reactions of Singly-Reduced Ethylene Carbonate in Lithium Battery Electrolytes: A Molecular Dynamics Simulation Study Using the ReaxFF*, J. Phys. Chem. A, 2012, 116, 2978-2985 (https://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*, Model. Simul. Mater. Sci. Eng. 2012, 20, 015002 (https://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*, J. Chem. Phys. 2013, 139, 044109 (https://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*, J. Chem. Phys. C, 2014, 118, 4967-4981 (https://dx.doi.org/10.1021/jp411015a)

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

Co.ff: (Co)

X.Q. Zhang, E. Iype, S.V. Nedea, 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*, J. Chem. Phys. C, 2014, 118, 6882-6886 (https://dx.doi.org/10.1021/jp500053u)

- Forcefield was generated using a Monte Carlo algorithm with simulated annealing.
- Branch: combustion.

CHONSFe.ff: (C/H/O/N/S/Fe)

E. Moerman, D. Furman, and D.J. Wales, *Development of ReaxFF Reactive Force Field for Aqueous Iron–Sulfur Clusters with Applications to Stability and Reactivity in Water*, J. Chem. Inf. Model. 2021, 61, 1204-1214 (https://dx.doi.org/10.1021/acs.jcim.0c01292)

- Reactive MD-force field for aqueous iron-sulfur clusters

CHONiHe.ff: (C/H/O/Ni/He)

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. Chem. Phys. C, 2010, 114, 4939-4949 (https://dx.doi.org/10.1021/jp9035056)

- Hydrocarbon chemistry on nickel surfaces
- Includes surface defect formation and partial substrate carburisation

CHONSMgPNaCuCl.ff: (C/H/O/N/S/Mg/P/Na/Cu/Cl)

S. Monti, C. Li, and V. Carravetta, *Reactive Dynamics Simulation of Monolayer and Multilayer Adsorption of Glycine on Cu(110)*, J. Phys. Chem. C, 2013, 117, 5221-5228 (https://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)

M.M. Islam, V.S. Bryantsev, and 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, 161, E3009-E3014 (https://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, 2780-2787 (https://dx.doi.org/10.1021/jp4121029)

- Interactions with water and Na+ were based on: J.C. Fogarty, H.M. Aktulga, A.Y. Grama, A.C.T. van Duin, and S.A. Pandit, *A reactive molecular dynamics simulation of the silica-water interface*, J. Chem. Phys. 2010, 132, 174704 (https://dx.doi.org/10.1063/1.3407433)
- Includes interactions between glycide and C/H/F.
- Includes Si-F bond, offdiagonal and angle parameters.
- Uses dummy Si-S bond parameters.
- Includes S-O-H parameters.
- Includes H-F bond and offdiagonal parameters.
- Includes Zr/O/H/C interactions.
- Branch: water.

TiClOH.ff: (C/H/O/N/S/Mg/P/Na/Ti/Cl/F)

S.Y. 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, 5655-5663 (https://dx.doi.org/10.1021/jp4031943)

- Adaptation/evolution of the TiOCHNCl.ff forcefield.
- 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, 7029-7039 (https://dx.doi.org/10.1021/jp300221j)

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

NiCHPt-2009.ff: (Ni/C/H/O/N/S/F/Pt/Cl)

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 (https://dx.doi.org/10.1021/jp9035056)

- Adaptation of the NiCH.ff forcefield with Ni-Pt interactions
- Training data has later been described in: 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, 16, 2797-2802 (https://dx.doi.org/10.1002/cphc.201500527)
- Branch: combustion.

LiS.ff: (Li/S)

M.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 (https://dx.doi.org/10.1039/C4CP04532G)

- Developed for and used to study Sulfur cathode behavior 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, Q. 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, 4039-4043 (https://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”
- Branch: combustion.

CHONSSiNaP.ff: (C/H/O/N/S/Si/Na/P)

B. 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, 12008-12016 (https://dx.doi.org/10.1021/jp5054277)

- Developed for studying carbon dioxide interactions with the ionic liquid tetrabutylphosphonium glycinate, including physical and chemical absorption.
- Glycinate utilizes dummy N-P parameters.

- Several lines from the valence angle block were referring to non-existent atoms from the atomic block and were therefore 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, 2156-2166 (https://dx.doi.org/10.1021/ct501027v)

- Used for studying Li/C systems with GCMC and MD
- Parameters were fitted using a training set consisting, among 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.

CHONSSiCaCsKSrNaMgAlCu.ff: (C/H/O/N/S/Si/Ca/Cs/K/Sr/Na/Mg/Al/Cu)

G.M. Psofogiannakis, 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, 6678-6686 (https://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.
- This forcefield is an extension of the H-ZSM-5 forcefield developed by K.L. Joshi, G. Psofogiannakis, A.C.T. van Duin, and S. Raman: *Reactive Molecular Simulations of Protonation of Water Clusters and Depletion of Acidity in H-ZSM-5 Zeolite*, Phys. Chem. Chem. Phys. 2014, 16, 18433-18441 (https://dx.doi.org/10.1039/C4CP02612H). All parameters (aside from Cu) are the same between both forcefields. The current forcefield is therefore also applicable to simulations of H-ZSM-5 zeolites.
- The Cu parameters were obtained 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 manuscript).
- 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 (https://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, Y.K. 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 (https://dx.doi.org/10.1039/C3CP51931G)

- Developed for peptide and protein simulations
- This forcefield is an extension of CHONSMgPNaCuCl.ff
- 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 (https://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)

S. Huygh, A. Bogaerts, A.C.T. van Duin, and E.C. Neyts, *Development of a ReaxFF reactive force field for intrinsic point defects in titanium dioxide*, Comp. Mat. Sci. 2014, 95, 579-591 (https://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.
- Based on TiOCHNCl.ff
- Branch: water.

LiSi.ff: (Li/Si)

A. Ostadhossein, E.D. Cubuk, G.A. Tritsaris, 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 (https://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, 7226-7236 (https://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, Y.K. Shin, A.C.T. van Duin, H. Fang, and Z.K. Liu, *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, 2015, 83, 102-112 (https://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, 13580-13589 (https://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, 571-580 (https://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*, Surf. Sci, 2016, 646, 253-260 (https://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.

CHONSFPtClNi.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, 16, 2797-2802 (https://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, 12561-12572 (https://dx.doi.org/10.1021/jp1080302)

- Forcefield designed for the study of laser-induced incandescence of soot
- Branch: combustion.

CHOSFClN.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, 885-895 (https://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)

J. Mueller and B. Hartke, *ReaxFF Reactive Force Field for Disulfide Mechanochemistry, Fitted to Multireference ab Initio Data;*, J. Chem. Theory Comput. 2016, 12, 3913-3925 (https://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)

S.J. Pai, B.C Yeoa, and S.S. Han, *Reactive force field for the improved design of liquid CBN hydrogen storage materials*, Phys. Chem. Chem. Phys. 2016, 18, 1818-1827 (https://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*, Surf. Sci., 2016, 645, 67-73 (https://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)

S. Hong and A.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, 9464-9474 (https://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, 31431-31440 (https://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. Bandosz, 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 (https://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)

S. Monti, V. Carravetta, and H. Ågren, *Simulation of Gold Functionalization with Cysteine by Reactive Molecular Dynamics*, J. Phys. Chem. Lett. 2016, 7, 272-276 (https://dx.doi.org/10.1021/acs.jpclett.5b02769)

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

HOSiAlLi.ff: (H/O/Si/Al/Li)

A. Ostadhossein, S.Y. Kim, E.D. Cubuk, Y. Qi, and A.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, 2114-2127 (https://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)

K. Yoon, A. Rahnamoun, J.L. Swett, V. Iberi, D.A. Cullen, I.V. Vlassiouk, 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, 8376-8384 (https://dx.doi.org/10.1021/acsnano.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)

R. Smith, K. Jolley, C. Latham, M. Heggie, A.C.T. van Duin, D. van Duin, and H. Wu, *A ReaXFF carbon potential for radiation damage studies*, Nucl. Instrum. Methods Phys. Res. B, 2017, 393, 49-53 (https://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)

R. 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, 6321-6333 (https://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/Eh)

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, 27128-27134 (https://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

CHOFeAlNiCuSCrSiGe.ff: (C/H/O/Fe/Al/Ni/Cu/S/Cr/Si/Ge)

Y. Zheng, S. Hong, G. Psofogiannakis, 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, 15848-15856 (https://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.
- Includes interactions with other oxides.

CHOAlGeX.ff: (C/H/O/Al/Ge)

Y. Zheng, S. Hong, G. Psofogiannakis, 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, 15848-15856 (https://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.
- Interactions with other oxides are included in CHOFeAlNiCuSCrSiGe.ff

Water2017.ff: (H/O)

W. Zhang and 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, 6021-6032 (https://dx.doi.org/10.1021/acs.jpcb.7b02548)

- Improved description of liquid water compared to the default water branch

HSMo.ff: (H/S/Mo)

A. Ostadhossein, 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, 631-640 (https://dx.doi.org/10.1021/acs.jpclett.6b02902)

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

CHON2017_weak.ff: (C/H/O/N/S/Mg/P/Na/Cu/Cl)

W. 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 (https://dx.doi.org/10.1021/acs.jpcb.8b01127)

- Retraining of the CHONSMgPNaCuCl_v2.ff force-field with 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)

H. Manzano, R.J.M. Pellenq, F.J. Ulm, M.J. Buehler, and A.C.T. van Duin, *Hydration of Calcium Oxide Surface Predicted by Reactive Force Field Molecular Dynamics*, Langmuir, 2012, 28, 4187-4197 (https://dx.doi.org/10.1021/la204338m)

- Hydration of a 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)

C. Ashraf and A.C.T. van Duin, *Extension of the ReaxFF Combustion Force Field toward Syngas Combustion and Initial Oxidation Kinetics*, J. Phys. Chem. A, 2017, 121, 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)

A. Vashisth, C. Ashraf, W. Zhang, C.E. Bakis, and A.C.T. van Duin, *Accelerated ReaxFF Simulations for Describing the Reactive Cross-Linking of Polymers*, J Phys Chem A, 2018, 122, 6633-6642 (https://dx.doi.org/10.1021/acs.jpca.8b03826)

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

CH_aromatics.ff: (C/H)

Q. Mao, Y. Ren, K.H. Luo, and A.C.T. van Duin, *Dynamics and kinetics of reversible homo-molecular dimerization of polycyclic aromatic hydrocarbons*, J. Chem. Phys. 2017, 147, 244305 (https://dx.doi.org/10.1063/1.5000534)

- Forcefield for polycyclic aromatic hydrocarbons

CuSCH.ff: (C/H/O/S/Cu/Cl)

J. 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. Chem. Phys. 2017, 147, 244305 (https://dx.doi.org/10.1021/acs.jpcb.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)

S. Monti, M. Pastore, C. Li, F. De Angelis, and V. 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, 2787-2796 (https://dx.doi.org/10.1021/acs.jpcc.5b11332)

- Forcefield for indoline adsorption on anatase

CHFe.ff: (C/H/Fe)

M.M. Islam, C. Zou, A.C.T. van Duin, and S. 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://dx.doi.org/10.1039/C5CP06108C)

- Forcefield for hydrogen adsorption on iron carbides

CHOGe.ff: (C/H/O/Ge)

N. Nayir, A.C.T. van Duin, and S. Erkoc, *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, 1208-1218 (https://dx.doi.org/10.1021/acs.jpcc.8b08862)

- Created by extending the training set from CHOFeAlNiCuSCrSiGe.ff 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, 23515-23527 (https://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, W. Sun, L. Deng, J. Du, T. Liang, S.B. Sinnott, and A.C.T. van Duin, *Development of a ReaxFF Reactive Force Field for NaSiOx/Water Systems and Its Application to Sodium and Proton Self-Diffusion*, J. Phys. Chem. C, 2018, 122, 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, 2125-2141 (https://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

CHON-2019.ff: (C/H/O/N)

M. Kowalik, C. Ashraf, B. Damirchi, D. Akbarian, S. Rajabpour, and A.C.T. van Duin, *Atomistic Scale Analysis of the Carbonization Process for C/H/O/N-Based Polymers with the ReaxFF Reactive Force Field*, J. Phys. Chem. B, 2019, 123, 5357-5367 (https://dx.doi.org/10.1021/acs.jpcb.9b04298)

- Improved force field for C/H/O/N chemistry based on DFT data with focus on N2 formation kinetics and its interactions with polymer-associated radicals formed during the carbonization process.
- Study of polymer (PAN, PBO) conversion to graphite
- The original file contained NaNs for all the 19th atomic parameters, which were set to 0 here

CuZr.ff: (Cu/Zr)

H.S. Huang, L.Q. Ai, A.C.T. van Duin, M. Chen, and Y. J. Lu, *ReaxFF reactive force field for molecular dynamics simulations of liquid Cu and Zr metals*, J. Chem. Phys. 2019, 151, 094503 (https://dx.doi.org/10.1063/1.5112794)

- Developed for MD on thermophysical properties of liquid Cu and Zr metals
- Optimized by fitting to DFT calc. on equations of state for bulk crystal structures and surface energies
- Represents structural characteristics and diffusion behaviors of elemental Cu and Zr up to high-temperature liquid regions.

ZrYOHVac.ff: (Zr/Y/O/H)

A.D. Mayernick, M. Batzill, A.C.T. van Duin, and M.J. Janika, *A reactive force-field (ReaxFF) Monte Carlo study of surface enrichment and step structure on yttria-stabilized zirconia*, Surf. Sci. 2010, 604, 1438-1444 (https://dx.doi.org/10.1016/j.susc.2010.05.006)

- Designed to investigate surface segregation in yttria-stabilized zirconia (YSZ)
- Parameterized with DFT energies describing surface energy as a function of yttrium lattice position
- Used for MC simulated annealing to sample structural configurations of flat YSZ (111) and vicinal YSZ (111) stepped surfaces

Ag-e.ff: (Ag/El)

B. Evangelisti, K.A. Fichthorn, and A.C.T. van Duin, *Development and initial applications of an e-ReaxFF description of Ag nanoclusters*, J. Chem. Phys. 2020, 153, 104106 (https://dx.doi.org/10.1063/5.0018971)

- This forcefield uses the ACKS2 charge model
- This forcefield is an eReaxFF forcefield
- Parameterized for Ag nanoclusters with 20 atoms or less
- Accurately reproduces the 2D-3D transition observed between the Ag5 and Ag7 clusters

ZrYONiH.ff: (Zr/Y/O/Ni/H)

S.S. Liu, L.C. Saha, A. Iskandarov, T. Ishimoto, T. Yamamoto, Y. Umeno, S. Matsumura and M. Koyama, *Atomic structure observations and reaction dynamics simulations on triple phase boundaries in solid-oxide fuel cells*, Commun. Chem. 2019, 2, 48 (https://dx.doi.org/10.1038/s42004-019-0148-x)

- Forcefield developed for Triple Phase Boundary (TPB) metal, oxide and gas simulations
- Solid oxide fuel cell anode research

CHONSi.ff: (C/H/O/N/Si)

Y. Wang, Y. Shi, Q. Sun, K. Lu, M. Kubo, and J. Xu, *Development of a Transferable ReaxFF Parameter Set for Carbon- and Silicon-Based Solid Systems*, J. Phys. Chem. C, 2020, 124, 10007-10015 (https://dx.doi.org/10.1021/acs.jpcc.0c01645)

- Developed for the research of Carbon/Silicon-based solid lubricants

CuCHO.ff: (Cu/C/O/H)

W. Zhu, H. Gong, Y. Han, M. Zhang, and A.C.T. van Duin, *Development of a Reactive Force Field for Simulations on the Catalytic Conversion of C/H/O Molecules on Cu-Metal and Cu-Oxide Surfaces and Application to Cu/CuO-Based Chemical Looping*, J. Phys. Chem. C, 2020, 124, 12512-12520 (https://dx.doi.org/10.1021/acs.jpcc.0c02573)

- Developed for the Cu-metal surface catalysis system

CHONSSiNaP-tribology.ff: (C/H/O/N/S/Si/Na/P)

D.C. Yue, T.B. Ma, Y.Z. Hu, J. Yeon, A.C.T. van Duin, H. Wang, and J. Luo, *Tribochemistry of Phosphoric Acid Sheared between Quartz Surfaces: A Reactive Molecular Dynamics Study*, J. Phys. Chem. C, 2013, 117, 25604-25614 (https://dx.doi.org//10.1021/jp406360u)

- Designed for studying friction coefficients in the silica/phosphoric acid system
- Extension of the model from J. Quenneville, R.S. Taylor, and A.C.T. van Duin, *Reactive Molecular Dynamics Studies of DMMP Adsorption and Reactivity on Amorphous Silica Surfaces*, J. Phys. Chem C, 2010, 114, 18894-18902 (https://dx.doi.org/10.1021/jp104547u) using additional Si/O/H parameters from J.C. Fogarty, H.M. Aktulga, A.Y. Grama, A.C.T. van Duin, and S.A. Pandit, *A reactive molecular dynamics simulation of the silica-water interface*, J. Chem. Phys. 2010, 132, 174704, (https://dx.doi.org/10.1063/1.3407433)

SiOHv2.ff: (Si/O/H)

N. Nayir, A.C.T. van Duin, and S. Erkoc, *Development of the ReaxFF Reactive Force Field for Inherent Point Defects in the Si/Silica System*, J. Phys. Chem. A, 2019, 123, 4303-4313 (https://dx.doi.org/10.1021/acs.jpca.9b01481)

- The supporting information was missing 3 general parameters, these have been filled in using the SiOH.ff data

- Redeveloped parameters for Si/O/H interactions, based on J.C. Fogarty, H.M. Aktulga, A.Y. Grama, A.C.T. van Duin, and S.A. Pandit, *A reactive molecular dynamics simulation of the silica-water interface*, J. Chem. Phys. 2010, 132, 174704, (https://dx.doi.org/10.1063/1.3407433)
- Enables MD simulations of Si/SiO2 interfaces and O diffusion in bulk Si at high temps, in particular with respect to point defect stability and migration

CHONSZr.ff: (C/H/O/N/S/Zr)

S. Dwivedi, M. Kowalik, N. Rosenbach, D.S. Alqarni, Y.K. Shin, Y. Yang, J.C. Mauro, A. Tanksale, A.L. Chaffee, and A.C.T. van Duin, *Atomistic Mechanisms of Thermal Transformation in a Zr-Metal Organic Framework, MIL-140C*, J. Phys. Chem. Lett. 2021, 12, 177-184 (https://dx.doi.org/10.1021/acs.jpclett.0c02930)

- Developed for studying thermal decomposition of a Zr-MOF (MIL-140C) using MD

CHONSMgPNaTiClFKLi.ff: (C/H/O/N/S/Mg/P/Na/Ti/Cl/F/K/Li)

K. Ganeshan, Yun K. Shin, N.C. Osti, Y. Sun, K. Prenger, M. Naguib, M. Tyagi, E. Mamontov, D. Jiang, and A.C.T. van Duin, *Structure and Dynamics of Aqueous Electrolytes Confined in 2D-TiO2/Ti3C2T2 MXene Heterostructures*, ACS Appl. Mater. Interfaces, 2020, 12, 58378-58389 (https://dx.doi.org/10.1021/acsami.0c17536)

- Developed for exploring the heterostructure of 2D lepidocrocite-type TiO2 (2D-TiO2) and hydroxylated or O-terminated Ti3C2 MXene in aqueous electrolytes using MD simulations and elastic/quasielastic neutron scattering techniques.

CeO.ff: (Ce/O)

P. Broqvist, J. Kullgren, M.J. Wolf, A.C.T. van Duin, and K. Hermansson, *ReaxFF Force-Field for Ceria Bulk, Surfaces, and Nanoparticles*, J. Phys. Chem. C, 2015, 119, 13598-13609 (https://dx.doi.org/10.1021/acs.jpcc.5b01597)

- Developed for stoichiometric ceria (CeO2) and partially reduced ceria (CeO2-x)
- Usage: The parameters have been tested for static calculations of CeO2 and partially reduced CeO(2-x). Use the in-cell approach (detailed in the paper) when calculating reaction energies.
- Warning: Note that elemental potentials taken from alloy descriptions may not work well for the pure species. This is particularly true if the elements were fit for compounds instead of being optimized separately. As with all interatomic potentials, please check to make sure that the performance is adequate for your problem.
- Note from authors: After publication, we have found additional false local minima. In particular one involving a short Ce-O bond (approx. 1.89 Ã) occurring in partially reduced ceria systems. This is problematic as it gives the wrong dynamic behavior. Attempts to heal this deficiency so far destroy the good performance regarding the ordering of the surface vacancy energies on the (111) surface. Therefore, it is recommended to keep track of the bond distances when analyzing the output.

InCH-2020.ff: (C/H/In)

S. Rajabpour, Q. Mao, N. Nayir, J.A. Robinson, and A.C.T. van Duin, *Development and Applications of ReaxFF Reactive Force Fields for Group-III Gas-Phase Precursors and Surface Reactions with Graphene in Metal–Organic Chemical Vapor Deposition Synthesis*, J. Phys. Chem. C, 2021, 125, 10747-10758 (https://dx.doi.org/10.1021/acs.jpcc.1c01965)

- Developed to investigate the MOCVD gas-phase reactions of In film growth from trimethylindium (TMIn) precursors, as well as the surface interactions of TMIn with graphene.

GaCH-2020.ff: (C/H/Ga)

S. Rajabpour, Q. Mao, N. Nayir, J.A. Robinson, and A.C.T. van Duin, *Development and Applications of ReaxFF Reactive Force Fields for Group-III Gas-Phase Precursors and Surface Reactions with Graphene in Metal–Organic Chemical Vapor Deposition Synthesis*, J. Phys. Chem. C, 2021, 125, 10747-10758 (https://dx.doi.org/10.1021/acs.jpcc.1c01965)

- Developed to investigate the MOCVD gas-phase reactions of Ga film growth from trimethylgallium (TMGa) precursors, as well as the surface interactions of TMGa with graphene.

HONSiF.ff: (H/O/N/Si/F)

D.H. Kim, S.J. Kwak, J.H. Jeong, S. Yoo, S.K. Nam, Y. Kim, and W.B. Lee, *Molecular Dynamics Simulation of Silicon Dioxide Etching by Hydrogen Fluoride Using the Reactive Force Field*, ACS Omega, 2021, 6, 16009-16015 (https://dx.doi.org/10.1021/acsomega.1c01824)

- Developed for a Si/O/H/F system to perform etching simulations of SiO2 with HF.

CsPbI.ff: (I/Pb/Cs)

M. Pols, J.M. Vicent-Luna, I. Filot, A.C.T. van Duin, and S. Tao, *Atomistic Insights Into the Degradation of Inorganic Halide Perovskite CsPbI3: A Reactive Force Field Molecular Dynamics Study*, J. Phys. Chem. Lett. 2021, 12, 5519-5525 (https://dx.doi.org/10.1021/acs.jpclett.1c01192)

- Developed for molecular dynamics simulations of the phase instability and the defect-induced degradation in the CsPbI3 perovskite.

CHOLiAlTiP.ff: (C/H/O/Li/Al/Ti/P)

Y.K. Shin, M.Y. Sengul, A.S.M. Jonayat, W. Lee, E.D. Gomez, C.A. Randall, and A.C.T. van Duin, *Development of a ReaxFF reactive force field for lithium ion conducting solid electrolyte LiAlTi(PO4)3 (LATP)*, Phys. Chem. Chem. Phys. 2018, 20, 22134-22147 (https://dx.doi.org/10.1039/C8CP03586E)

- Developed for NASICON-type Li1+xAlxTi2-x(PO4)3 (LATP) materials, which is a promising solid-electrolyte that may enable all-solid-state lithium-ion batteries.

WSHAlO.ff: (W/S/H/Al/O)

N. Nayir, Y.K. Shin, Y. Wang, M.Y. Sengul, D. Reifsnyder Hickey, M. Chubarov, T.H. Choudhury, N. Alem, J. Redwing, V.H. Crespi, and A.C.T. van Duin, *A ReaxFF Force Field for 2D-WS2 and its Interaction with Sapphire*, J. Phys. Chem. C, 2021, 125, 17950-17961 (https://dx.doi.org/10.1021/acs.jpcc.1c03605)

- Designed to capture the most essential features of a WS2 thin film, such as the 2H → 1T displacive phase transition, S-vacancy migration, and the energetics of various point and line defects, e.g., ripplocations in a WS2 monolayer.

SiAlMgO.ff: (Si/Al/Mg/O)

J. Yeon, S.C. Chowdhury, C.M. Daksha, and J.W. Gillespie Jr., *Development of Mg/Al/Si/O ReaxFF Parameters for Magnesium Aluminosilicate Glass Using an Artificial Neural Network-Assisted Genetic Algorithm*, J. Phys. Chem. C, 2021, 125, 18380-18394 (https://dx.doi.org/10.1021/acs.jpcc.1c01190)

- Developed to describe Mg/Al/Si/O interactions in S-glass and other magnesium aluminosilicate (MAS) glass compositions.
- The training set includes the density functional theory data of the energy response of various Mg/Al/Si/O crystals during volumetric expansion and compression and Mg migration inside Mg/Al/Si/O crystals.

CHOSMoNiLiBFPN-2.ff: (C/H/O/S/Mo/Ni/Li/B/F/P/N)

Y. Liu, Q. Sun, P. Yu, Y. Wu, L. Xu, H. Yang, M. Xie, T. Cheng, and W.A. Goddard III, *Effects of High and Low Salt Concentrations in Electrolytes at Lithium–Metal Anode Surfaces Using DFT-ReaxFF Hybrid Molecular Dynamics Method*, J. Phys. Chem. Lett. 2021, 12, 2922-2929 (https://dx.doi.org/10.1021/acs.jpclett.1c00279)

- Extension of CHOSMoNiLiBFPN.ff with parameters for (fluorosulfonyl)imide anions.

NiCr.ff: (Ni/Cr)

Y.K. Shin, Y. Gao, D. Shin, and A.C.T. van Duin, *Impact of three-body interactions in a ReaxFF force field for Ni and Cr transition metals and their alloys on the prediction of thermal and mechanical properties*, J. Phys. Chem. C, 2021, 125, 17950-17961 (https://dx.doi.org/10.1021/acs.jpcc.1c03605)

- After introducing three-body interaction parameters to the metal force field, ReaxFF can successfully predict experimental elastic constants of FCC Ni and BCC Cr at finite temperatures.

CHNOSSi.ff: (C/H/O/N/S/Si)

M.J. Buehler, A.C.T. van Duin, and W.A. Goddard III, *Multiparadigm Modeling of Dynamical Crack*

Propagation in Silicon Using a Reactive Force Field, Phys. Rev. Lett. 2006, 96, 095505 (https://dx.doi.org/10.1103/PhysRevLett.96.095505)

- Study of dynamic cracking in a silicon single crystal in which the ReaxFF reactive force field.

CHONSSiGe_2016.ff: (C/H/O/N/S/Si/Ge)

J. Wen, T. Ma, W. Zhang, G. Psofogiannakis, A.C.T. van Duin, L. Chen, L. Qian, Y. Hu, and X. Lu, *Atomic insight into tribochemical wear mechanism of silicon at the Si/SiO2 interface in aqueous environment: Molecular dynamics simulations using ReaxFF reactive force field*, Appl. Surf. Sci. 2016, 390, 216-223 (https://dx.doi.org/10.1016/j.apsusc.2016.08.082)

- Study of tribochemical wear of silicon at the Si/SiO2 interface in aqueous environment.

RuNH.ff: (Ru/N/H)

S.Y. Kim, H.W. Lee, S.J. Pai, and S.S. Han, *Activity, Selectivity, and Durability of Ruthenium Nanoparticle Catalysts for Ammonia Synthesis by Reactive Molecular Dynamics Simulation: Size Effect*, ACS Appl. Mater. Interfaces, 2018, 10, 26188-26194 (https://dx.doi.org/10.1021/acsami.8b05070)

- Study of ammonia synthesis from nitrogen and hydrogen over Ru nanoparticle
- During force-field fitting the following quantities were considered: equations of states of various Ru crystals, surface formation energies for various Ru surfaces, adsorption energies of N and H atoms on Ru surfaces, various reaction pathways (N2 dissociation, H diffusion, and NH3 formation) on Ru surfaces, and Ru-N and Ru-H bond dissociations in several nonperiodic systems.

Water-ereaxff2.ff: (O/H/El/Eh/Ho)

S. Bertolini and Timo Jacob, *Valence energy correction for electron reactive force field*, J. Comput. Chem. 2022, 43, 870 (https://dx.doi.org/10.1002/jcc.26844)

- Extension of the eReaxFF method with explicit electron dependence in the three-body terms.
- Demonstration of this extension in parametrized for hydrogen and oxygen interactions, including water and the related ions (H3O+ and OH-).

CHONSMgPNaCuClTi.ff: (C/H/O/N/S/Mg/P/Na/Cu/Cl/Ti)

D. Hou, M. Feng, J. Wei, Y. Wang, A.C.T. van Duin, and K.H. Luo, *A reactive force field molecular dynamics study on the inception mechanism of titanium tetraisopropoxide (TTIP) conversion to titanium clusters*, Chem. Eng. Sci. 2022, 252, 117496 (https://dx.doi.org/10.1016/j.ces.2022.117496)

- New Ti/C/H/O ReaxFF force field based on CHON2017_weak.ff.
- Study of pyrolysis of titanium tetraisopropoxide.

CHONSSiCaCsKSrNaMgAlClIFLiX.ff: (C/H/O/N/S/Si/Ca/Cs/K/Sr/Na/Mg/Al/Cl/I/F/Li)

M.G. Muraleedharana, R. Herz-Thyhsenb, J.C. Deweyb, J.P. Kaszubab, and A.C.T. van Duin, *Understanding the chemistry of cation leaching in illite/water interfacial system using reactive molecular dynamics simulations and hydrothermal experiments.*, Acta Materialia 2020, 186, 564-574 (https://dx.doi.org/10.1016/j.actamat.2019.12.059)

- This work combines CaSiAlO.ff and CHOCsKNaClIFLi.ff force fields to obtain a transferable H/O/Si/Al/K force field for clay minerals containing potassium counterions.
- Study of potassium leaching from the illite clay mineral.

CHOSMoNiAuTi.ff: (C/H/O/S/Mo/Ni/Au/Ti)

Q. Mao, Y. Zhang, M. Kowalik, N. Nayir, M. Chandross, and A.C.T. van Duin, *Oxidation and hydrogenation of monolayer MoS2 with compositing agent under environmental exposure: The ReaxFF Mo/Ti/Au/O/S/H force field development and applications*, Front. Nanotechnol. 2022, 4, 1034795 (https://dx.doi.org/10.3389/fnano.2022.1034795)

- The force field is applied to simulations of the effect of the Ti dopant on the oxidation/hydrogenation behaviors of MoS2 surface.

RuH.ff: (Ru/H)

C. Onwudinanti, M. Pols, G. Brocks, V. Koelman, A.C.T. van Duin, T. Morgan,and S. Tao, *A ReaxFF molecular dynamics study of hydrogen diffusion in ruthenium - the role of grain boundaries*, J. Phys. Chem. C, 2022, 126, 5950 (https://dx.doi.org/10.1021/acs.jpcc.1c08776)

- This work makes use of reactive molecular dynamics simulations to study the influence of imperfections in a Ru film on the behavior of H.
- For the Ru/H system, a ReaxFF force field which reproduces structures and energies obtained from quantum-mechanical calculations was parametrized.
- Molecular dynamics simulations have been performed with the newly developed force field to study the effect of tilt and twist grain boundaries on the overall diffusion behavior of H in Ru.

MgO.ff: (Mg/O)

F. Fiesinger, D. Gaissmaier, M. van den Borg, J. Bessner, A.C.T. van Duin, and T. Jacob, *Development of a Mg/O ReaxFF Potential to describe the Passivation Processes in Magnesium-Ion Batteries*, Chem. Sus. Chem. 2023, 16, e202201821 (https://dx.doi.org/10.1002/cssc.202201821)

- A Mg/O ReaxFF force field potential was developed that enables large-scale simulations of Mg/O systems.
- Insights into the ongoing passivation mechanism are provided by investigating the reaction processes of the Mg anode in an O2 atmosphere.

LiSiC.ff: (Li/Si/C)

S.B. Olou'ou Guifo, J.E. Mueller, D. van Duin, M.K. Talkhoncheh, and A.C.T. van Duin, *Development and Validation of a ReaxFF Reactive Force Field for Modeling Silicon-Carbon Composite Anode Materials in Lithium-Ion Batteries*, J. Phys. Chem. C, 2023, 127, 2818-2834 (https://dx.doi.org/10.1021/acs.jpcc.2c07773)

- A forcefield developed for SiC anode material for lithium-ion batteries.

NiAl.ff: (Ni/Al)

W. Du, X. Fan, H. Li, D. Zhai, and Y, Liu, *Development of a Ni–Al reactive force field for Ni-based superalloy: revealing electrostatic effects on mechanical deformation*, J. Mater. Res. Technol. 2023, 24, 4454-4467 (https://dx.doi.org/10.1016/j.jmrt.2023.04.038)

- A forcefield developed for Ni-Al superalloys

CHONSSiGeGaAg.ff: (C/H/O/N/S/Si/Ge/Ga/Ag)

F. Niefind, Q. Mao, N. Nayir, M. Kowalik, J.J. Ahn, A.J. Winchester, C. Dong, R.A. Maniyara, J.A. Robinson, A.C.T. van Duin, and S. Pookpanratana, *Watching (De)Intercalation of 2D metals in Epitaxial Graphene: Insight to Role of Defects*, Small, 2023, 11, 2306554 (https://dx.doi.org/10.1002/smll.202306554)

- Study of de-intercalation of 2D Ag and Ga metals sandwiched between bilayer graphene and SiC.

CHOZn.ff: (C/H/O/Zn)

S.S. Han, S.H. Choib, and A.C.T. van Duin, *Molecular dynamics simulations of stability of metal-organic frameworks against H2O using the ReaxFF reactive force field*, Chem. Commun. 2010, 46, 5713-5715 (https://dx.doi.org/10.1039/C0CC01132K)

- Study of the hydrolysis reactions and water stability of MOFs

CHONBAlSiCl.ff: (C/H/O/N/B/Al/Si/Cl)

N. Uene, T. Mabuchi, M. Zaitsu, S. Yasuhara, A.C.T. van Duin, and T. Tokumasu, *Reactive Force Field Molecular Dynamics Studies of the Initial Growth of Boron Nitride Using BCl3 and NH3 by Atomic Layer Deposition*, J. Phys. Chem. C, 2024, 128, 1075-1086 (https://dx.doi.org/10.1021/acs.jpcc.3c06704)

- A new forcefield for atomic layer deposition of boron nitride thin film growth using BCl3 and NH3

IBrPbCs.ff: (I/Br/Pb/Cs)

M. Pols, A.C.T. van Duin, S. Calero, and S. Tao, *Mixing I and Br in Inorganic Perovskites: Atom-*

istic Insights from Reactive Molecular Dynamics Simulations, J. Phys. Chem. C, 2024, 128, 4111-4118 (https://dx.doi.org/10.1021/acs.jpcc.4c00563)

- Extension of a CsPbI3 force-field
- Optimized using ParAMS
- Can accurately reproduce finite-temperature effects of the material, such as phase transitions between various bulk phases of the inorganic perovskites.

HOAlSiNaK.ff: (H/O/Al/Si/Na/K)

Y. Zhang, X. Liu, A.C.T. van Duin, X. Lu, and E.J. Meijer, *Development and validation of a general-purpose ReaxFF reactive force field for earth material modeling*, J. Chem. Phys. 2024, 160, 094103 (https://dx.doi.org/10.1063/5.0194486)

- Parametrized using DFT data
- Intended for high temperature and pressure conditions

CHOMnLiFNSP.ff: (C/H/O/Mn/Li/F/N/S/P)

M.K. Talkhoncheh, H. Ghods, M. Doosthosseini, J. Silberberg, I. Kyprianou, and A.C.T. van Duin, *Development of the ReaxFF Reactive Force Field for Li/Mn/O Battery Technology with Application to Design Self-Healing Cathode Electrolyte Interphase*, J. Phys. Chem. C, 2024, 128, 6538-6550 (https://dx.doi.org/10.1021/acs.jpcc.3c07242)

- Derived from the Li/Mn/C/H/O force field by W.Y. Tsai, S.B. Pillai, K. Ganeshan, S. Saeed, Y. Gao, A.C.T. van Duin, V. Augustyn, and N. Balke, *Effect of Electrode/Electrolyte Coupling on Birnessite (δ-MnO2) Mechanical Response and Degradation*, ACS Appl. Mater. Interfaces, 2023, 15, 26120-26127 (https://dx.doi.org/10.1021/acsami.3c02055)
- Parametrized using DFT data

CHOCrNiFLiNaK.ff: (C/H/O/Cr/Ni/F/Li/Na/K)

H. Arkoub, S. Dwivedi, A.C.T. van Duin, and M. Jin, *A reactive force field approach to modeling corrosion of NiCr alloys in molten FLiNaK salts*, Appl. Surf. Sci. 2024, 655, 159627 (https://dx.doi.org/10.1016/j.apsusc.2024.159627)

- The original paper describes systems used for force field training in detail
- The Ni/Cr/F part was parametrized using small metal fluoride clusters and F on surface

CHAPTER

EIGHT

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

8.1 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 ehader 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.
       cov r3;Elp;Heat inc.;n.u.;n.u.;n.u.;n.u.
       ov/un;val1;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;13corr;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.

8.2 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, 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)

Note: The `SCM developer notes` contain very detailed information about all the ReaxFF equations, including some information that concerns SCM's implementation of ReaxFF. That SCM-specific information can be ignored.

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

continues on next page

Table 8.1 – continued from previous page

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
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

continues on next page

Table 8.2 – continued from previous page

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
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^pipi	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 (RvdW[C]*RvdW[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.

When setting the off-diagonal van der Waals energy to a negative number, the mixing rule is used to derive this parameter from the atomic values.

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

CHAPTER

NINE

TROUBLESHOOTING AND WARNINGS

9.1 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.jpclett.9b02810).

9.2 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*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.

CHAPTER

TEN

REQUIRED CITATIONS

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

10.1 General References

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. E.J. Baerends, N.F. Aguirre, N.D. Austin, J. Autschbach, F.M. Bickelhaupt, R. Bulo, C. Cappelli, A.C.T. van Duin, F. Egidi, C. Fonseca Guerra, A. Förster, M. Franchini, T.P.M. Goumans, T. Heine, M. Hellström, C.R. Jacob, L. Jensen, M.V. Krykunov, E. van Lenthe, A. Michalak, M. Mitoraj, J. Neugebauer, V.P. Nicu, P.H.T. Philipsen, H. Ramanantoanina, R. Rüger, G. Schreckenbach, M. Stener, M. Swart, J.M. Thijssen, T. Trnka, L. Visscher, A.L. Yakovlev, S.J.A. van Gisbergen, *The Amsterdam Modeling Suite*, Journal of Chemical Physics 162, 162501 (2025) (https://doi.org/10.1063/5.0258496)
4. ReaxFF 2026.1, SCM, Theoretical Chemistry, Vrije Universiteit, Amsterdam, The Netherlands, https://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
5. Cite the reference for the *force field file* (page 21).

See also the citations for the AMS Driver.

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

10.2 Special ReaxFF features

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)

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

CHAPTER

ELEVEN

FAQ

11.1 What's the difference between ReaxFF in AMS and the standalone program?

In AMS2020, ReaxFF integrated with the AMS driver is the default. This gives consistent input for different modules and enables new properties through the central driver. It also helps users more easily switch between modules and use ReaxFF in multi-layer hybrid simulations.

Some ReaxFF features have not yet been ported to the integrated ReaxFF, and can be used from the *standalone ReaxFF* (page 15).

11.2 Can I use GPU acceleration in ReaxFF?

No.

11.3 Which ReaxFF force field should I use?

Click on i next to Force field input in ReaxFF Input to see which force fields are included with ReaxFF. Alternatively, open **$AMSHOME/atomicdata/ForceFields/ReaxFF/Readme**, which also contains the original references and sometimes a short description. The list of *currently available ReaxFF force fields* (page 21) are available in the documentation.

You are strongly advised to check the original publications to see how the force field has been trained and to what type of systems it has been applied.

If no force field is available for your elements, check the literature or parametrize it yourself, see the other FAQs.

11.4 I can not find a published ReaxFF force field for my atoms, how to make a new force field?

This is hard work, which takes quite a bit of training and experience.

The ReaxFF parameters are typically trained against DFT data and parameters should be optimized for all atom types in your system. In principle, parameters are transferable across systems, but including additional atoms requires also to include new interactions with all new element combinations. This is not trivial, but we try to help you with our ParAMS ReaxFF parametrization (https://www.scm.com/product/params/) tools.

RxFF consulting (https://www.rxffconsulting.com/) offers consulting services for optimizing force field parameters for new materials.

11.5 What does 'Force field problem: missing bonds' mean?

There are two elements in your simulation box for which no bonded parameters are present in the force field file. Please check the description and the paper on the *ReaxFF force field page* (page 21).

You can find more info on which bond, angle, and dihedral terms exist, and which ones are missing by using the checkreaxffforcefield.py utility:

```
$AMSBIN/startpython $AMSHOME/scripting/standalone/reaxff/checkreaxffforcefield.py /
↪path/to/yourreaxff.ff
```

You'll probably find that this force field was not designed for the elements you want to study. Perhaps there is another force field more suitable for your application.

You may try to our reparametrize the force field.

11.6 Is a ReaxFF force field available for elements X, Y, Z?

In the GUI: build a ReaxFF input with these elements X, Y, and Z, and click on the folder icon next to Force field:. A list of force fields included in the AMS/ReaxFF distribution that contain these atom types will be shown. If force fields are available, consult the Readme (click 'i') to check the publication to make sure this is the force field for your application.

If no force field shows up in the list, no suitable force field is available in your distribution. Use google or web of knowledge to find out if a ReaxFF force field exists for your application. If it does, and the force field is printed in the supporting information, you can add the ReaxFF force field file (see *FAQ* (page 57)) to the existing ones in the distribution.

Note that not all terms may be available for all element combinations. To get more insight in which force field terms are available, use the python ReaxFF force field checking tool:

```
$AMSBIN/startpython $AMSHOME/scripting/standalone/reaxff/checkreaxffforcefield.py /
↪path/to/yourreaxff.ff
```

You can find a description of the general structure of the force field file and the parameters from the original ReaxFF documentation (https://www.scm.com/wp-content/uploads/ReaxFF-users-manual-2002.pdf).

11.7 What is the origin of the elements in the force field file not described in the publication?

We try to include as much information on the origin of parameters in *the ReaxFF manual* (page 21) as well as in the GUI help files.

Many published ReaxFF force fields are building upon a previous set of parameters, and so only the elements studied in that paper are being refined, and the other parameters are just kept in place. You could try to trace back the origin of some of these parameters by looking at the existing force fields and finding out where the same parameters for a particular element also appear. Any force field that has matching atomic parameters might have some information about the origins of the parameters in the corresponding publication or in the information in the force field description file.

However, you need to be careful by just combining and using elements / parameters from different force fields. See also the FAQ about ReaxFF parameter transferability. You should also be aware that certain bonded terms may not be available for a particular unpublished element and/or combination of elements, so you are strongly advised to check this with our ReaxFF force field checking tool: **$AMSHOME/scripting/checkreaxffforcefield.py**. The original ReaxFF documentation (https://www.scm.com/wp-content/uploads/ReaxFF-users-manual-2002.pdf) describes the general structure and correspondence of the columns with the parameters.

11.8 How transferable are ReaxFF parameters to different simulations (other molecules or environment) from the ones they were developed for?

In general the parameters are quite transferable, but some forcefields were developed for specialized cases such as explosives research (high pressure). It is good practice to scan through the publication of the forcefield (you can find the information by clicking the "i" button behind the forcefield) before using it extensively. It is also wise to do some testing simulations to see if your structures are not falling apart or folding into weird geometries.

11.9 How do I export the ReaxFF trajectory to Gromacs or pdb?

This is most easily done from the GUI using the **File → Export Trajectory As:** option in AMSJobs. You can export as Gromacs, PDB trajectory, or xmol file. For the .gro export you will get an additional dialogue window where you can include the timestep and the velocities.

Alternatively, you can use the scripting tool amsreport, e.g.

```
amsreport yourreaxff.rxkf -r gro-t0.00025 > yourreaxff.gro
```

The options for amsreport in your AMS distribution are displayed if you type

```
amsreport -h
```

11.10 Why are bonds still being broken or formed during a non-reactive ReaxFF simulation?

During a non-reactive ReaxFF simulation the connection table is determined only once at the beginning of a simulation and is then kept fixed. Other than this the same ReaxFF procedure with the same forces and energy expressions is used. Therefore, if the system is far from equilibrium, or if the temperature is too high, bonds may still be broken or formed.

You can also think about simulating the system at zero Kelvin with a strong thermostat to try and get your system to the nearest local minimum without changing the bonds too much.

11.11 Can you run a simulation with any combination of elements available in the ReaxFF force field?

This depends on what parameters are available in the force field file. A ReaxFF force field consists of some generic parameters, a number of atomic parameters (1 set for every atom type), bond parameters (combination of 2 atom types), angle parameters (combination of 3 atom types), dihedral parameters (combination of 4 atom types) and possibly hydrogen bond parameters (see original ReaxFF documentation (https://www.scm.com/wp-content/uploads/ReaxFF-users-manual-2002.pdf) for more details).

If a force field has elements X, Y an Z it means that it contains atomic parameters for X, Y and Z. However, it does not necessarily contain all combinations of the bond/angle/dihedral parameters. For example, X-X, Y-Y, Z-Z, X-Y and X-Z might have bond parameters, but Y-Z could be left out. This means that Y and Z should not be used together in the simulation, as their interaction is not defined.

To get more insight in which terms are available in a ReaxFF force field, use the python ReaxFF force field checking tool: **$AMSHOME/scripting/checkreaxffforcefield.py**

11.12 What is the difference between ReaxFF and the ReaxFF force fields?

ReaxFF consists of two parts: the program and the force field files:

– The ReaxFF program is an implementation of the ReaxFF forcefield equations (see the *Required citations ReaxFF page* (page 51) for the original papers). – The ReaxFF force field files contain the parameters needed by the force field equations when running your simulation, they consist of 5 or 6 parts (see original ReaxFF documentation (https://www.scm.com/wp-content/uploads/ReaxFF-users-manual-2002.pdf) for more details):

- generic parameters
- atom parameters (per element)
- atom pairs / bond parameters (combination of two elements)
- angle parameters (combination of three elements)
- dihedrals (combination of four elements)
- and sometimes hydrogen bonds (per element)

A ReaxFF force field is build using a training set (see other FAQs) and is usually targeted for a specific simulation and typically includes about 4 to 12 elements, as the number of parameters scales to the 4th power with the number of elements included. Because ReaxFF uses pair/angle/dihedral parameters, it is not possible to simply combine two forcefield files.

The AMS GUI can tell you if a force field is available for the elements in your simulation (see other FAQs), but it will not be able to tell if the force field is conditioned for your specific simulation type. For this you will have to check the publication of the force field (doi link is usually included in the Readme file or the first line of the force field file)

11.13 How do I use a ReaxFF force field I saw in a publication?

The AMS implementation of ReaxFF still takes the original format. If a publication has the parameters printed in the supporting information in native format, just copy that data and save it as a file, e.g. YourNewReaxFF.ff, in **$AMSHOME/atomicdata/ForceFields/ReaxFF**. Then you can start using that force field by selecting it in the GUI, by clicking **other** after you've clicked the folder icon next to **Force field:** in the input panel.

If the parameters are printed in tables in the manuscript, but not as a comprehensive SI file, you can still compile your own ReaxFF force field file from this data in the same original ReaxFF format.

It is advisable to use the checkreaxffforcefield.py script in **$AMSHOME/scripting/** to check your force field. If you have modified or downloaded a force field you may want to clean it up:

Open a shell in a terminal with AMS settings loaded. Then run the rxffutil tool (https://www.scm.com/doc.2024/OldReaxFF/Miscellaneous.html#the-rxffutil-utility)

```
rxffutil reformat < your_ff.ff
```

The resulting cleaned up ReaxFF force field is stored in a file 'ffield'.

11.14 Which thermostat and damping constant should I choose?

For the NHC thermostat/MTK barostat, the simulation samples the correct ensemble no matter what the damping time is set to, but it is recommended to set the damping time to roughly correspond to the correlation time of the system (how long it takes for the system to "forget" a disturbance). This is 2-3 picoseconds in liquid water, up to a couple hundred fs in solids. Setting it any longer doesn't improve the accuracy of the system anymore, just makes the thermostatting/barostatting less efficient (taking longer to settle).

Berendsen thermostats/barostats only approximate the correct ensemble and this approximation is the worse the shorter the damping time. It is thus crucial to set the damping time as high as practical to still reach the target value in acceptable time. Especially for the Berendsen thermostat, setting the damping time too low is known to result in severe equipartition artifacts (all kinetic energy is transferred from vibrations into rotational degrees of freedom, leading to the so-called "flying ice cube problem" (https://en.wikipedia.org/wiki/Flying_ice_cube)).

Setting the **damping constant/relaxation time** to a lower value means more aggressive thermostatting/barostatting. The system will be driven to reach the target temperature/pressure faster, which may be necessary if it starts far from equilibrium or if there's something in the system releasing or consuming a lot of energy (a chemical reaction). However, using a short relaxation time may also lead to artifacts (e.g. rapid changes of the volume by an aggressive barostat may disturb the structure of a condensed-phase system). Conversely, setting the relaxation time too high will make the thermostat/barostat very weak, affecting the system only minimally but also taking a lot of time to reach the target temperature/pressure.

The computational cost of any thermostat/barostat in AMS doesn't depend on the damping at all.

See also the webinar by Tomas Trnka on MD basics (https://www.youtube.com/watch?v=XhPIp3sDZTA) (slides (https://www.scm.com/wp-content/uploads/MD-basics.pdf))

11.15 Can I simulate ions with ReaxFF?

It is possible to constrain the net charge of a particular atom or molecule to a particular value, this can be done in the GUI under Model→Charge Constraints.

For the old standalone ReaxFF, charge constraints are defined by putting lines like the following into the “geo” file:

```
MOLCHARGE firstAtom lastAtom netCharge
```

where firstAtom and lastAtom define the range of atoms to be constrained (inclusive, numbering starts from 1). An unfortunate limitation of this approach is that all atoms in the system need to be covered by one of the MOLCHARGE lines because the ranges need to be continuous, this often requires some reordering of the atoms to be possible.

As an example, let’s say there are two ions that we want to constrain to +2 charge:

```
MOLCHARGE 1 1 2.0
MOLCHARGE 2 2 2.0
MOLCHARGE 3 1000 -4.0
```

We have moved the ions to the beginning of the system to be able to constrain the rest of the system and make sure the net charge of the whole simulation box is zero.

From on AMS2020, the AMS driver supports charge constraints for ReaxFF.

They can be defined in the ReaxFF Engine block as follows:

```
Engine ReaxFF
Charges
   Constraint Region=ion1 Charge=2.0
   Constraint Region=ion2 Charge=2.0
End
EndEngine
```

One thus only needs to put the ions into separate regions (for example using the GUI) and use the appropriate region names on the Constraint lines. There’s no need to reorder atoms here or to constrain the rest of the system (this happens naturally to keep the total charge at the value set in the System block).

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