

# Modeling chemical reactions with the Amsterdam Modeling Suite and the ReaxFF engine

## Chemical Vapor Deposition & Combustion



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# ReaxFF

## Reactive many-body interatomic potential

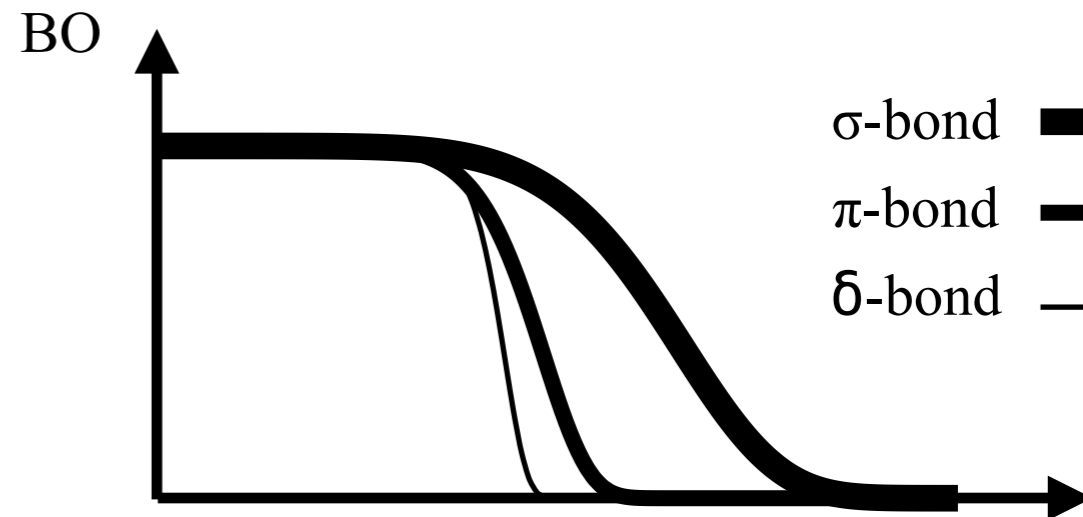
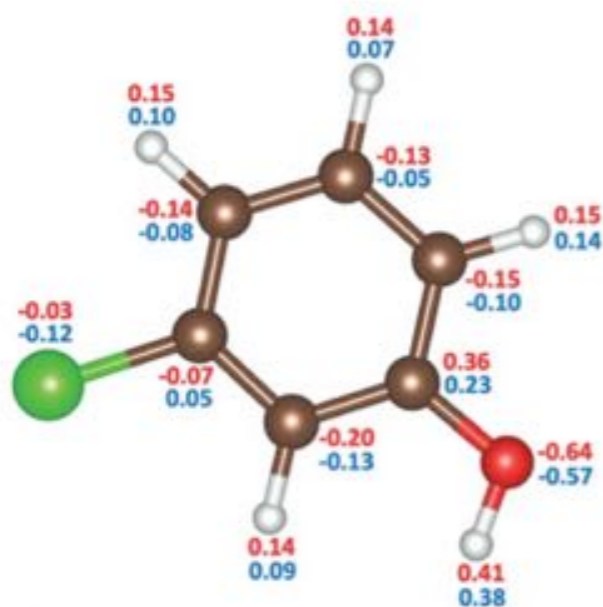
- The functional form

$$E_{pot} = \underbrace{E_{bond} + E_{ang} + E_{dih}} + E_{over/under} + E_{vdW} + E_{coul} + \dots$$

$$BO = \exp \left[ p_1 \left( \frac{r}{r_0} \right)^{p_2} \right] + \exp \left[ p_3 \left( \frac{r}{r_{0,\pi}} \right)^{p_4} \right] + \exp \left[ p_5 \left( \frac{r}{r_{0,\pi\pi}} \right)^{p_6} \right]$$

Learn more: <https://www.scm.com/product/reaxff/>

- Partial atomic charges: QEq



$$E(\{R_i\}\{Q_i\}) = \sum_i^N \left( \chi_i Q_i + \frac{1}{2} H_i Q_i^2 \right) + \sum_{i < j}^N Q_i Q_j J(R_{ij})$$

Van Duin et al. *J. Phys. Chem. A* 2001, 105, 41, 9596–9409

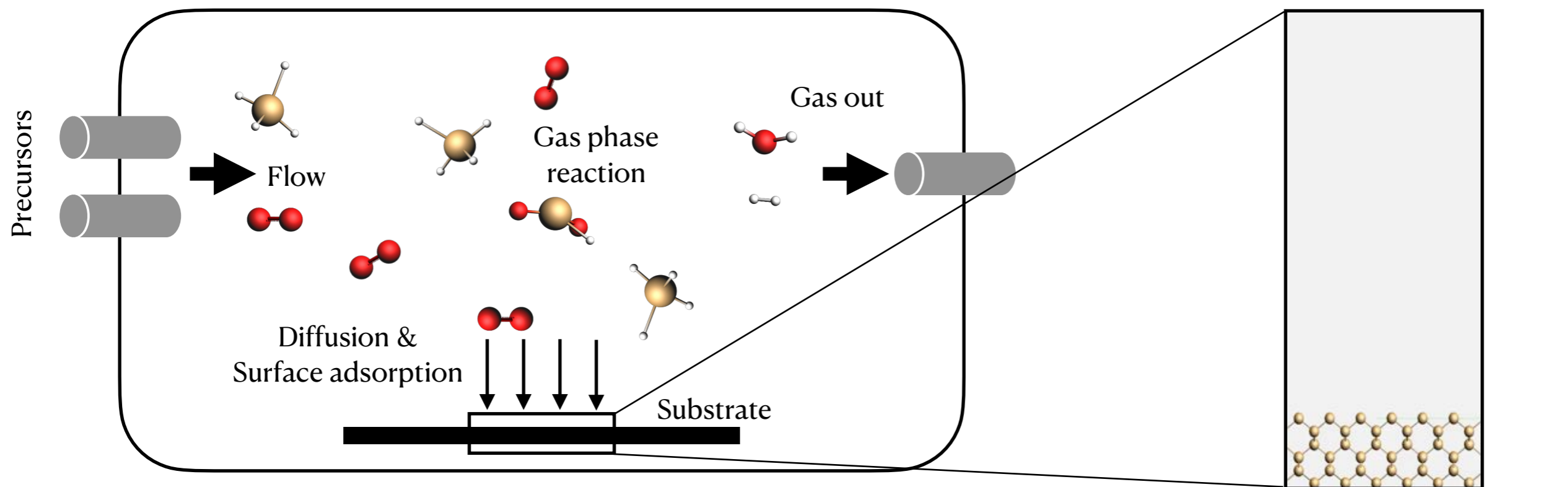
*J. Phys. Chem. A* 2003, 107, 19, 3803–3811

# Chemical vapor deposition

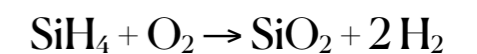
## Principle of CVD

- To produce thin films in semiconductor industry
- Wafer exposed to gas/plasma which react/decompose on the substrate

<https://www.scm.com/doc/Tutorials/MolecularDynamicsAndMonteCarlo/MoleculeGunSimulationCVD.html>



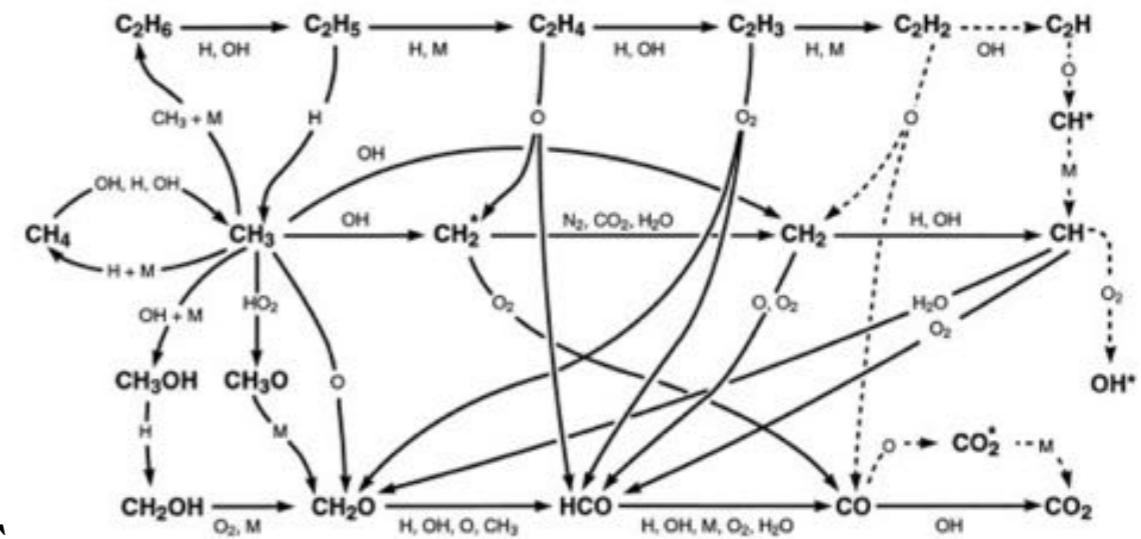
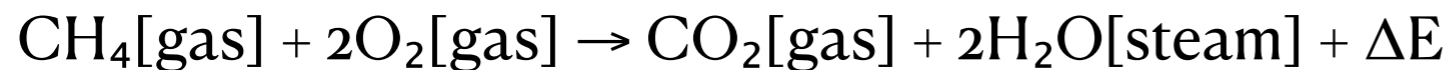
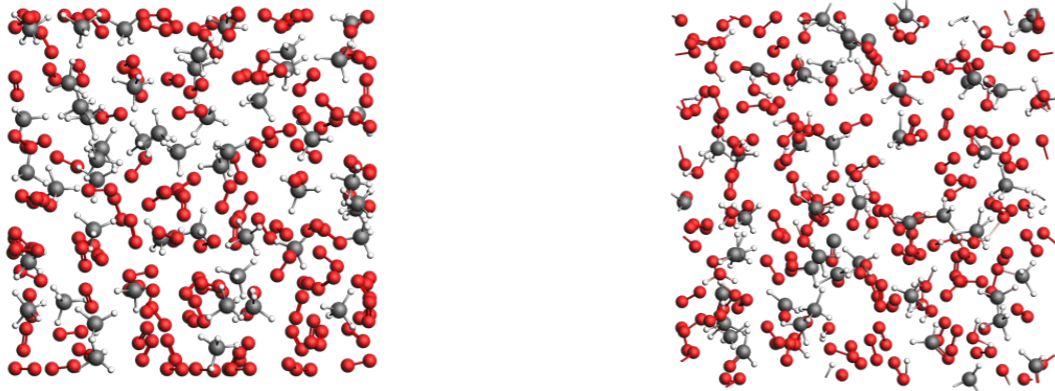
SiO<sub>2</sub> growth on Si substrate



# Combustion reaction

## Combustion of methane in oxygen

- High T MD simulation of O<sub>2</sub> + CH<sub>4</sub>



*H.N. Najm, P.H. Paul, C.J. Mueller and P.S. Wyckoff, Comb.Flame, 113, 312-332, 1998*

- ChemTraYzer2

| Reaction                     | Reaction Composition     | Order | Rate constant k (cm <sup>3</sup> /mol/s) | k lower bound | k upper bound | Number of events | Reaction event indices |
|------------------------------|--------------------------|-------|--|---------------|---------------|------------------|------------------------|
| 3000 + 3000CH2O => CH2O + O2 | HO2 + CH2O => CO2 + H2O2 | 2     | 1.847e+15                                | 1.280e+14     | 6.475e+15     | 1                | 175                    |
| 3046 + 200CH2O => CH2O + O   | HO + CH2O => CO2 + H2O   | 2     | 5.074e+15                                | 4.250e+14     | 5.894e+16     | 5                | 344                    |

| Index | Initial frame | Final frame | Initial time (fs) | Final time (fs) | Reactants | Products | Reactants composition | Products composition | Reactants atom indices      |
|-------|---------------|-------------|-------------------|-----------------|-----------|----------|-----------------------|----------------------|-----------------------------|
| 344   | 274           | 274         | 8875.0            | 8875.0          | CH4 + 2O2 | CH2O + O | HO + CH2O             | CO2 + H2O            | (248 412) + (31 83 248 376) |

