# 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

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

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

• Partial atomic charges: QEq





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

Van Duin et al. J. Phys. Chem. A 2001, 105, 41, 9396–9409 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



SiO2 growth on Si substrate



# **Combustion reaction**

### **Combustion of methane in oxygen**

• High T MD simulation of O2 + CH4





 $CH_4[gas] + 2O_2[gas] \rightarrow CO_2[gas] + 2H_2O[steam] + \Delta E$ 

H, OH H, OH H, OH H, M H, M H, OH H, OH H, M OH H, OH

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

• ChemTraYzer2

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https://www.scm.com/doc/Tutorials/MolecularDynamicsAndMonteCarlo/ChemTrayzer2.html https://www.scm.com/doc/Tutorials/MolecularDynamicsAndMonteCarlo/BurningIsooctane.html