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

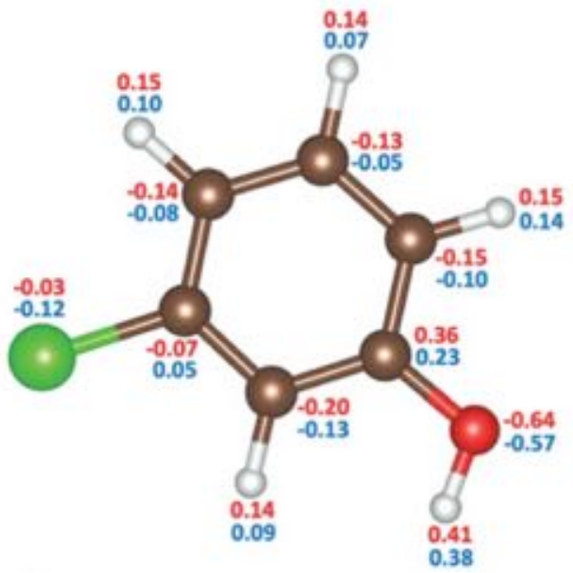
- The functional form

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

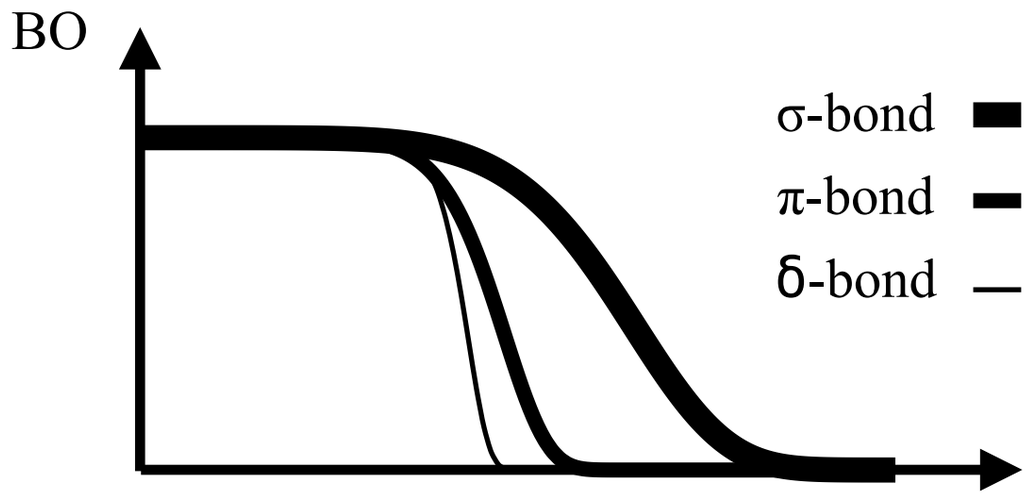
$$BO = exp\left[p_1 \left(\frac{r}{r_0}\right)^{p_2}\right] + exp\left[p_3 \left(\frac{r}{r_{0,\pi}}\right)^{p_4}\right] + exp\left[p_5 \left(\frac{r}{r_{0,\pi\pi}}\right)^{p_6}\right]$$

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

- Partial atomic charges: QEq



RSC Adv., 2021, 11, 2929



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

Van Duin et al. J. Phys. Chem. A 2001, 105, 41, 9396–9409
J. Phys. Chem. A 2003, 107, 19, 3803–3811

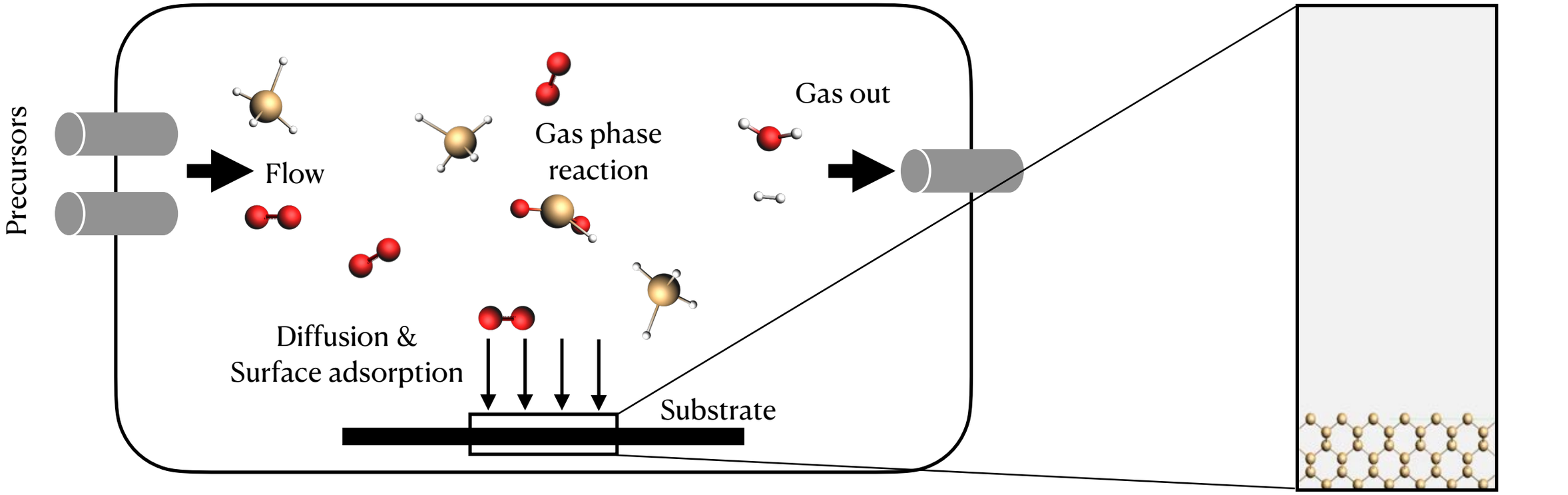
SCM

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



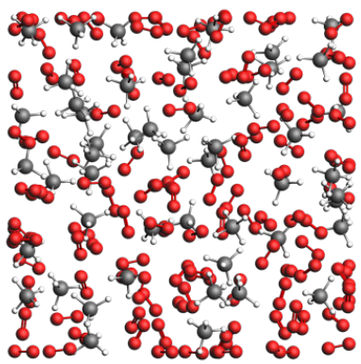
SiO_2 growth on Si substrate

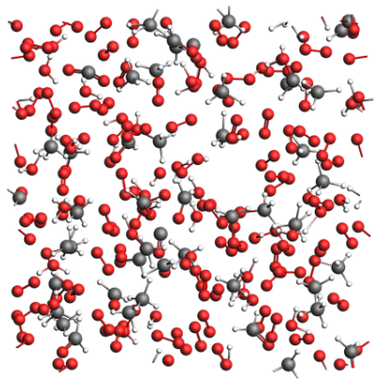
$$SiH_4 + O_2 \rightarrow SiO_2 + 2\,H_2$$

Combustion reaction

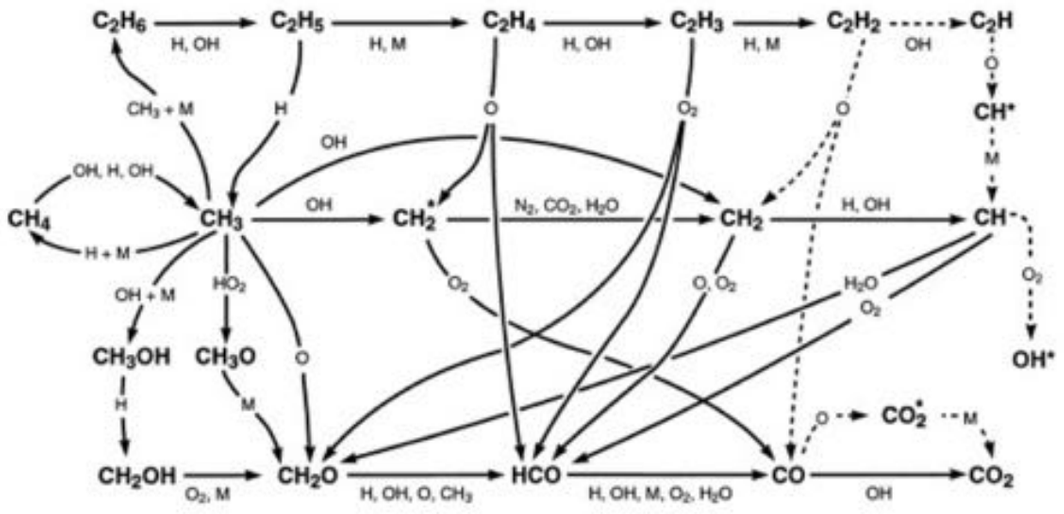
Combustion of methane in oxygen

- High T MD simulation of O2 + CH4



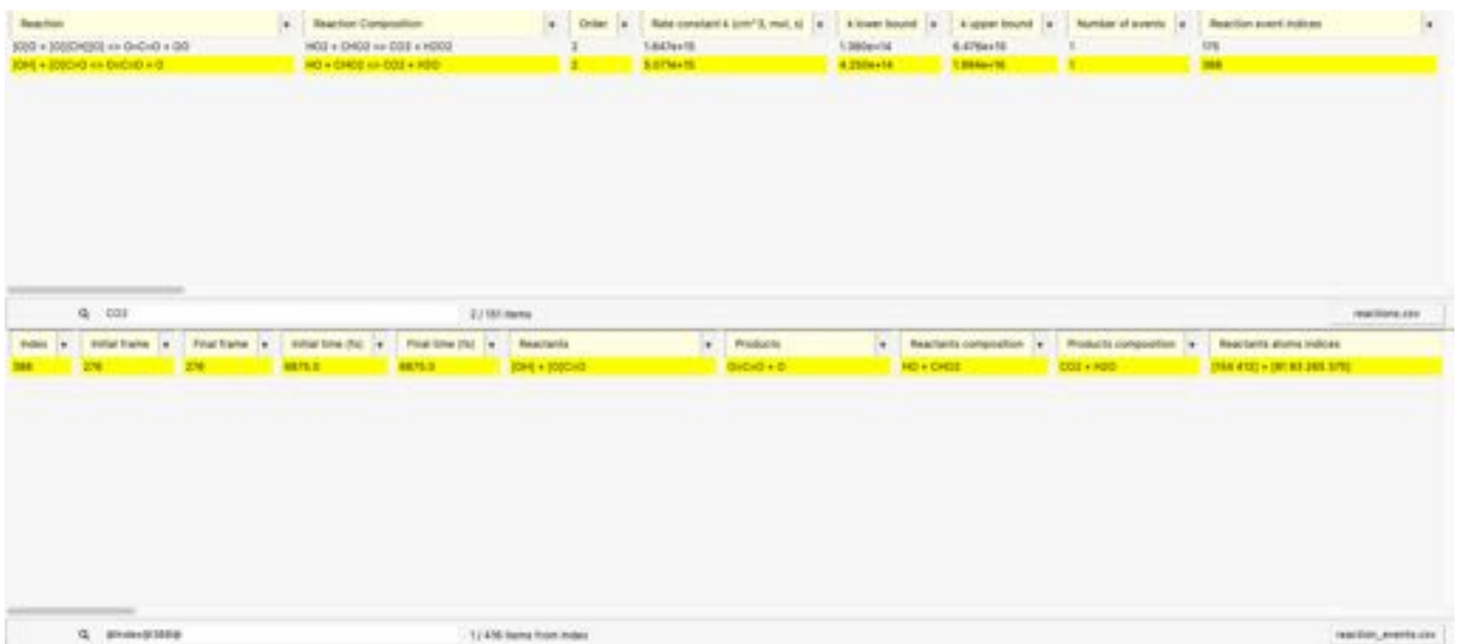


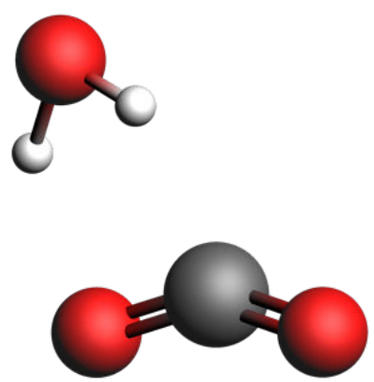
$$CH_4[gas] + 2O_2[gas] \rightarrow CO_2[gas] + 2H_2O[steam] + \Delta E$$



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

- ChemTraYzer2





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