Santiso Lab

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Lab Interests and Focus

Our group focuses on developing new methods to discover new materials and analyzing their chemical and physical properties using computer simulations. We try to study novel materials for applications as surfactants, surfaces for selective adsorption and crystallization enhancers/inhibitors.

We employ a variety of computational tools such as quantum chemistry and ab initio simulations, atomistic simulation methods and mesoscale group contribution techniques.

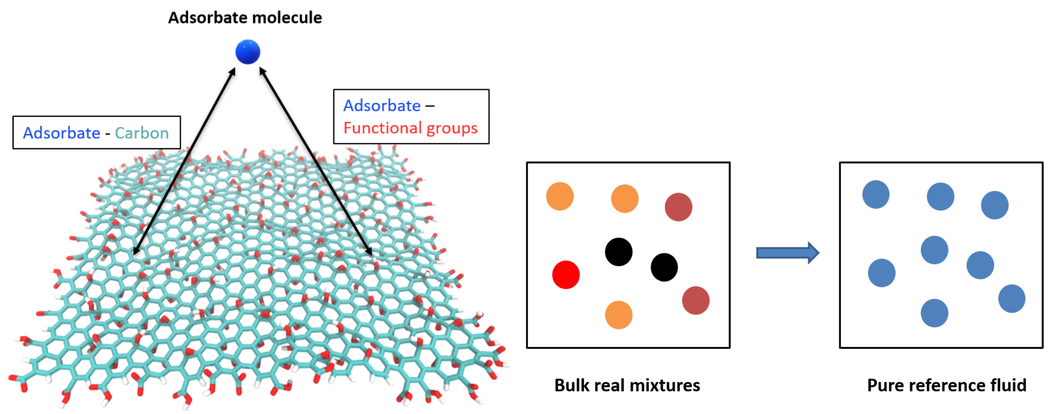
1) Molecular modeling of adsorption sites

Kaihang Shi

Experimentalists prefer theory, but why?

- Fast and convenient
- Needs less specialized knowledge

Conformal sites theory is an approximation of a real system where the free energy of mixture $A_{mixture} = A_{pure\ fluid} + T*S_{mixing}$

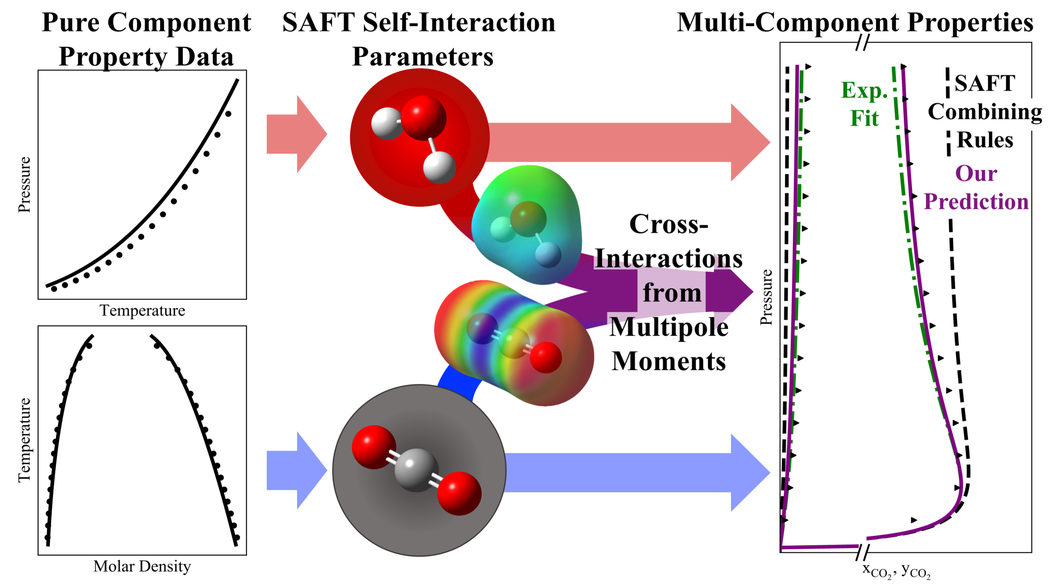


- **Goal: To develop a surface roughness theory which allows for chemical and geometric heterogeneity, while being flexible enough for arbitrary types of adsorption sites and site densities**
- **Level of Theory: Mesoscale**
- **Softwares/Packages: In-house Monte Carlo Program (FORTRAN)**

2) Forcefield development using DFT

Jennifer Clark

- **SAFT: Equation of state (EoS) based on first order perturbation of Helmholtz free energy**
- **Multipole moment calculations from DFT allow the inclusion of electrostatic dependencies in conventional forcefields**



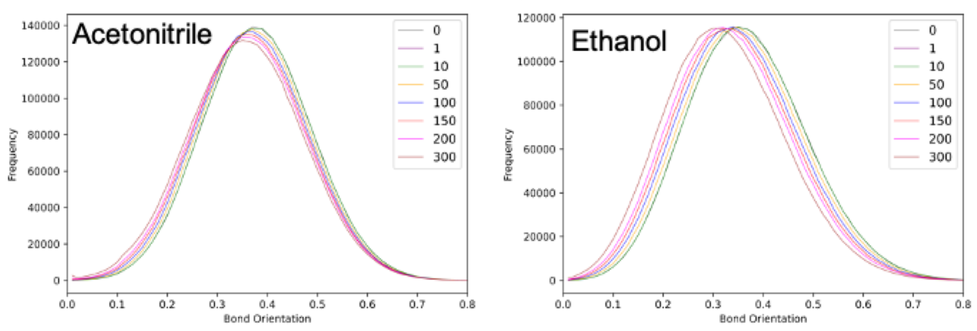
- **Goal: Develop and test an open-source software employing SAFT to generate component interaction parameters and electronic structure calculations to generate cross interaction parameters**
- **Level of theory: Quantum Chemical, Mesoscale**
- **Software/Packages: DESPASITO Python package, R.E.D. Server, Gaussian**

3) Order parameters and precipitate nucleation

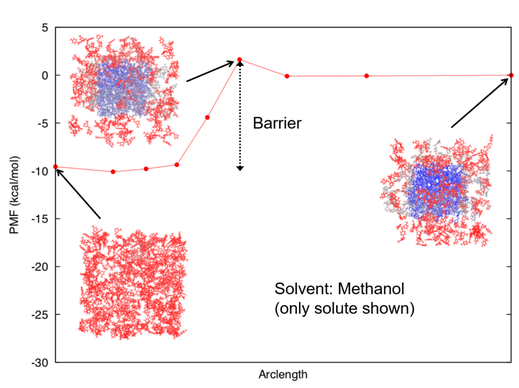
Daniel Cardenas Vasquez, Jake McKibbin

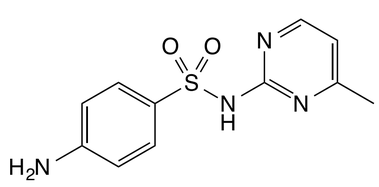
Order Parameters: Differentiates stable states from intermediates

Order Parameters for liquid solvents with Urea



- Correct prediction of stable states and intermediates for implicit solvent sulfamerazine at different crystallization conditions





Sulfamerazine: 3 known polymorphs, Crystallization induction time in methanol: 7200 min

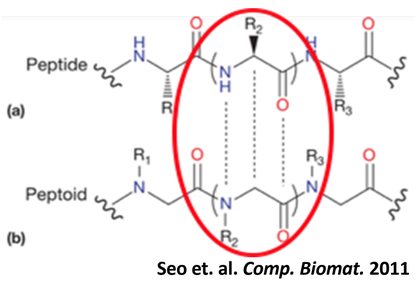
- **Goal: Use the developed order parameters to study explicit solvent nucleation of realistic models of drug molecules, selecting polymorphs and predicting properties**
- **Level of Theory: Atomistic, Mesoscale**
- **Softwares/Packages: LAMMPS, NAMD, AMBER**

4) Coarse Grained forcefield for peptoids

Rakshit Jain

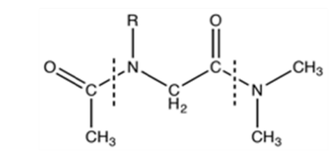
Peptoids vs Peptides

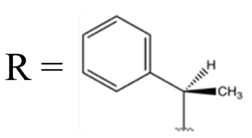
- Sidechain moved to backbone N atom
- No chiral α carbon
- No backbone H-bonding
- Protease resistant and thermally stable

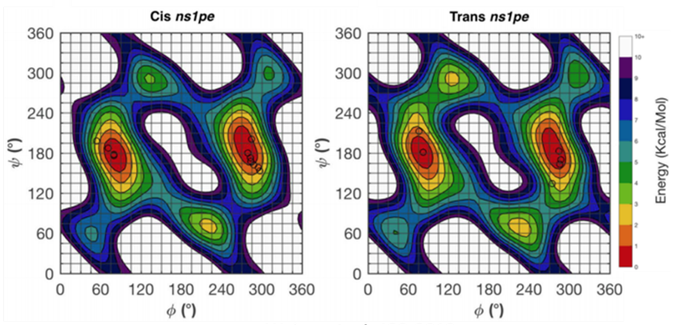


Seo et. al. *Comp. Biomat.* 2011

- **Atomistic Forcefield (NTOID in CHARMM General ForceField)**
- Performed atomistic simulations to fit parameters for a new atomtype in CGenFF
- Used Well-Tempered Metadynamics for accurate representation of free energy minima







Weiser et. al. *JCC*, 2019

- **Goal: Use top down (SAFT-γ) and bottom up (Relative Entropy) coarse graining to develop a Discontinuous Molecular Dynamics simulation forcefield for peptoids**
- **Level of Theory: Quantum Chemical, Atomistic, Mesoscale**
- **Softwares/Packages: GROMACS, NAMD, VOTCA, DESPASITO, VMD**