Developing Relationships between FW/OSDA orientation and Al siting

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Workflow

Objectives

1. Develop models to capture/describe the orientational preference a framework (FW) has for a particular organic structure directing agent (OSDA)

2. Identify FW/OSDA combinations that could influence Al ordering through preferential OSDA orientations.

3. Compute and compare organic and inorganic structure directing agent interactions with frameworks to identify consequences on Si/Al ratios

Plan of Attack

1. **What is the preferential orientational of a specific OSDA/Zeolite combination**

   (a) Develop a model to capture OSDA Orientations

   - Classical molecular dynamics (CMD) at very high temperatures ($T \geq 10,000$) to sample different possible orientation

   (b) Compute interaction energy (IE) of all FW and OSDA combinations (maybe free energies):

   - CHA and AEI with TMADA, DMDMP (isomers), and DEDMP (isomers)
     - include LTA and TMA?
   - Using CMD at 343 K (rigid framework)
   - Using density functional theory with dispersion (DFT-D3) (flexible framework)
     - Rigid Framework as well?

   (c) Evaluate orientation and positioning dependence of OSDA in FW

- Measure the orientation of an OSDA relative to some axis which encompases the cage the OSDA is in
- Measure the location of the OSDA center of mass is relative to the center of the zeolite cage

2. **What is the impact of Al siting with respect to OSDA orientation**

   (a) Using some preferred orientation(s)

   - Using the same technique developed by Sichi, run CMD on Al substituted FW and charged OSDA as in 1(a)
   - Refine using techniques in 1(b)

   (b) Compare relative energies (or IE?)

   - Is there a difference between AEI and CHA?

3. **What is the impact of co-caging (Relevent?)**

   (a) Charged or chargless model