Adsorption of Tetrafluoromethane on FAU Framework Zeolites – a Molecular Dynamics and Grand Monte Carlo Study

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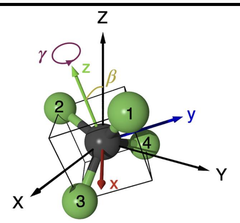
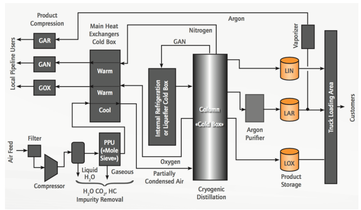
Research question: How can zeolite adsorbents be used to reduce emissions within the semiconductor industry?

CF_4 Atmospheric Pollution and Reclamation

- CF_4 is indispensable to chip manufacturing
- Global Warming Potential
  - 7000-9000 times CO_2
  - Lifetime of 50,000 years
- Cryogenic Distillation
  - High Pressure
  - Low Temperature
    - High energy cost





Molecular Dynamics

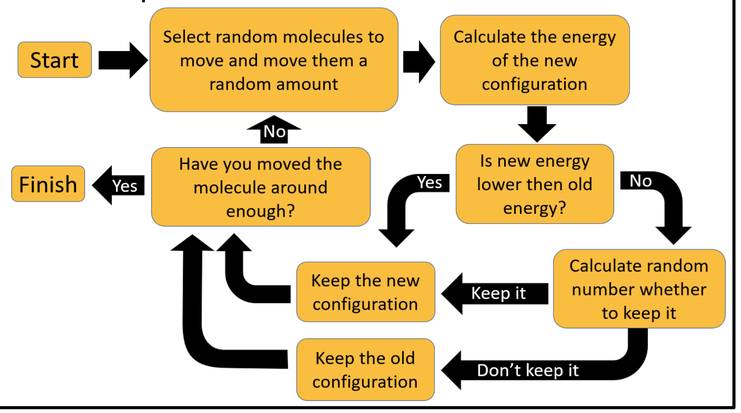
- Zeolite surfaces are large
  - Very expensive
  - Need Simple Process
- Molecular dynamics
  - Very cheap and simple process
  - Not realistic
    - Add relaxation step

Surface → Sorbate → ASAP (Automatic Surface Adsorbate Structure Provider) → Optimized Adsorbed Sorbate → Relaxed Adsorbed Sorbate

Grand Monte Carlo Simulations

- Stochastic method
  - More accurate to real life
  - More detail of equilibrium state
- Verifies adsorption
  - More expensive

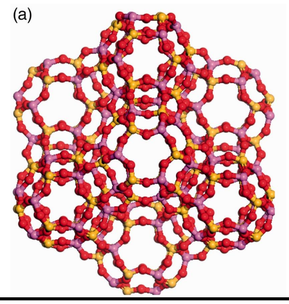
Zacros — Advanced lattice-KMC made easy



Zeolite 13X Adsorption Viability

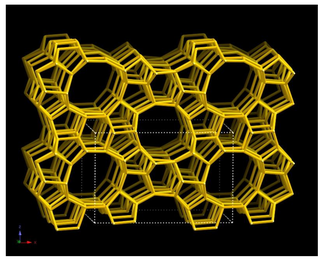
FAU zeolite surfaces were chosen because the literature showed zeolite 13X had high viability when removing CF_4 from nitrogen.

This was confirmed when the CF_4 remained adsorbed after the relaxation step



Future Work

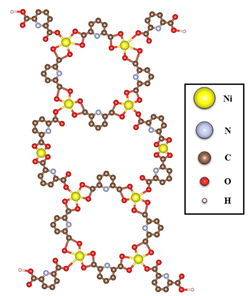
The Grand Monte Carlo portion still needs to be conducted as the Molecular Dynamics portion of the project took more time than originally anticipated.



Once completed this method could be expanded to any other zeolite framework in the database. MFI is a possibly promising structure due to its medium-sized pore structure.

Once other possible surfaces are identified and simulated the results will be verified further in the lab.

ASAP can be used for any porous surface including Metal-Organic Frameworks would be used to investigate surfaces of interest such as Ni-MOF and NH_2-Ni-MOF.



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