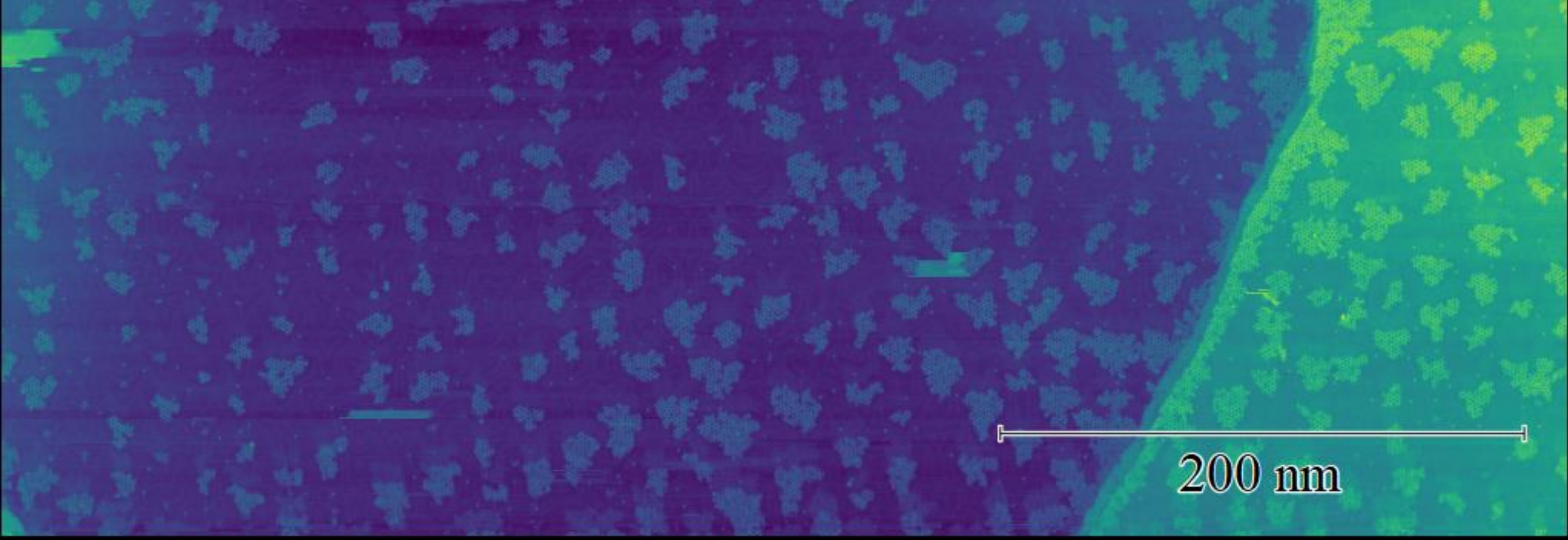


Kinetic Monte Carlo Simulations for Polymerization in 2 dimensions

Group Lunch - 2024-09-18 - Simon Briesenick

Motivation

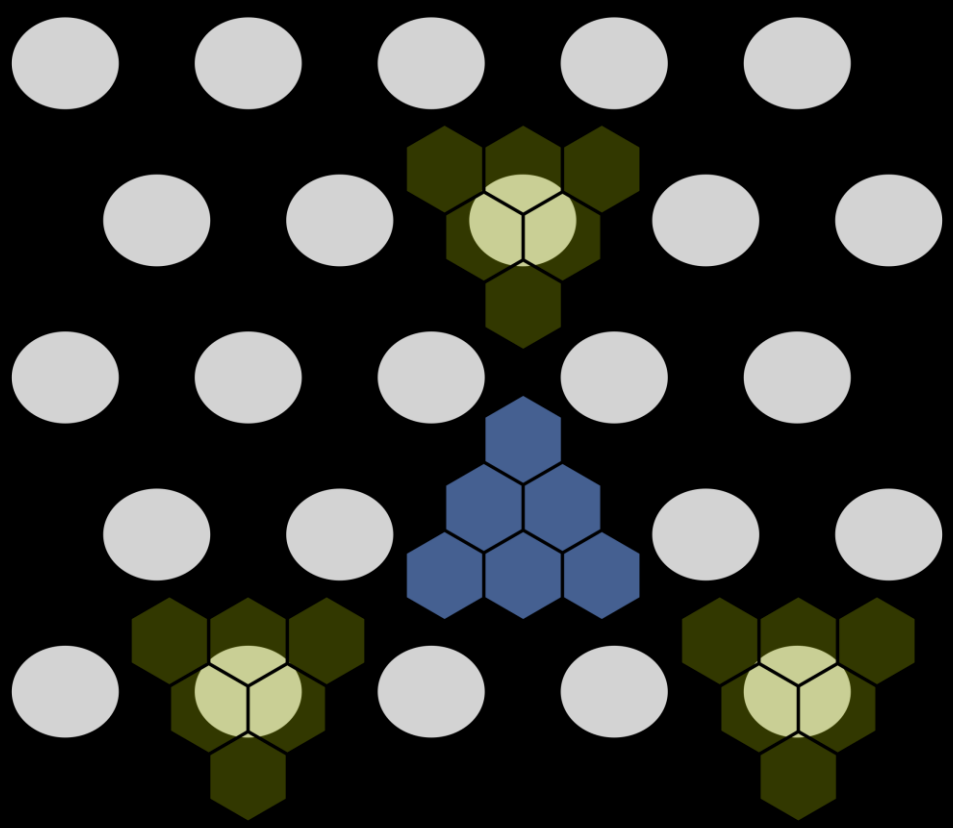
- Formation of 2D ordered networks is highly dependent on Monomer + Substrate interactions
  - Diffusion Barrier
  - Coupling Barrier
  - Rotational Barrier
  - Epitaxial Relationship

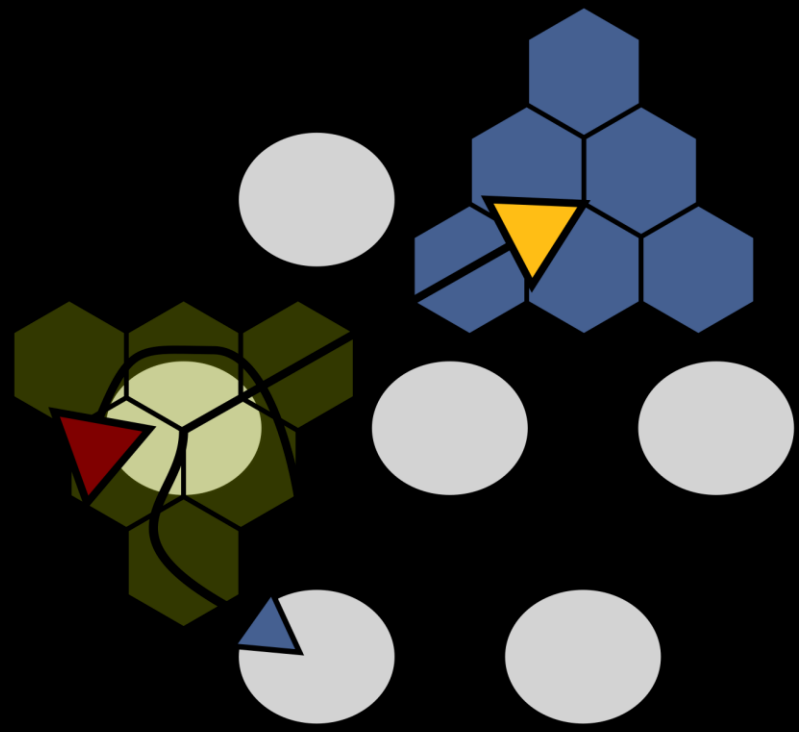
} Can be tweaked by material used, surface orientation, temperature, adatoms,

Can we use this model to better understand the reaction kinetics on different surfaces, and could we perhaps even extract the Monomer + Substrate interactions

Physical Model

Monomers appear on a hexagonal grid, and can diffuse, rotate, or couple to other monomers (if possible)





Implementation in Python

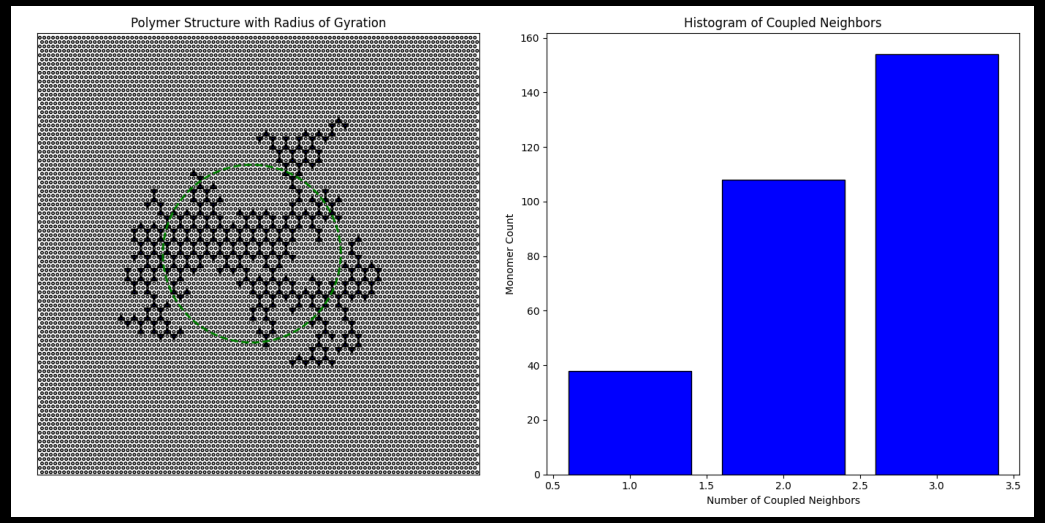
- Object-oriented approach with `Monomer` and `Lattice` classes
- Initialize lattice with single (fixed) monomer in the center.
  - 🔄 Add one monomer at a time on random position on the lattice
    - Each timestep, the (free) monomer can diffuse, rotate, and couple. The probability for each of these actions is given by an Arrhenius equation:

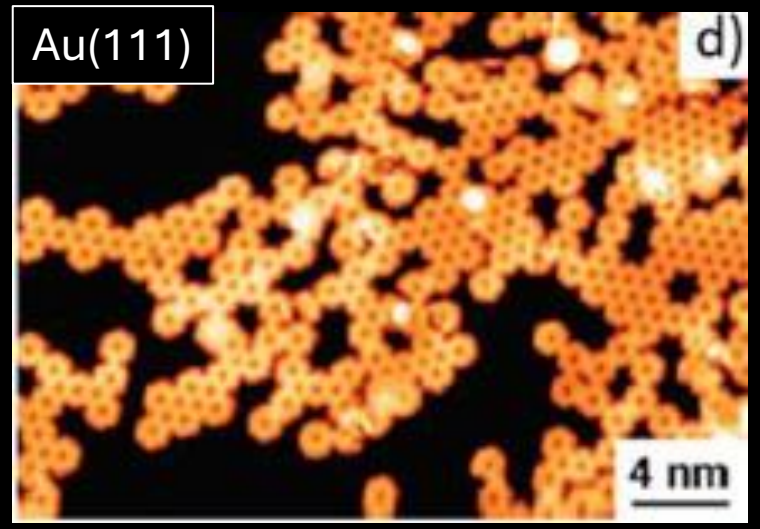
$$P^{d,r,c} = P_0^{d,r,c} \exp\left(-\frac{E^{d,r,c}}{k_B T}\right)$$

    - Run until new monomer has coupled to growing oligomer, and repeat.
    - A coupled monomer's probability for all actions is set to 0, i.e., they become immobile

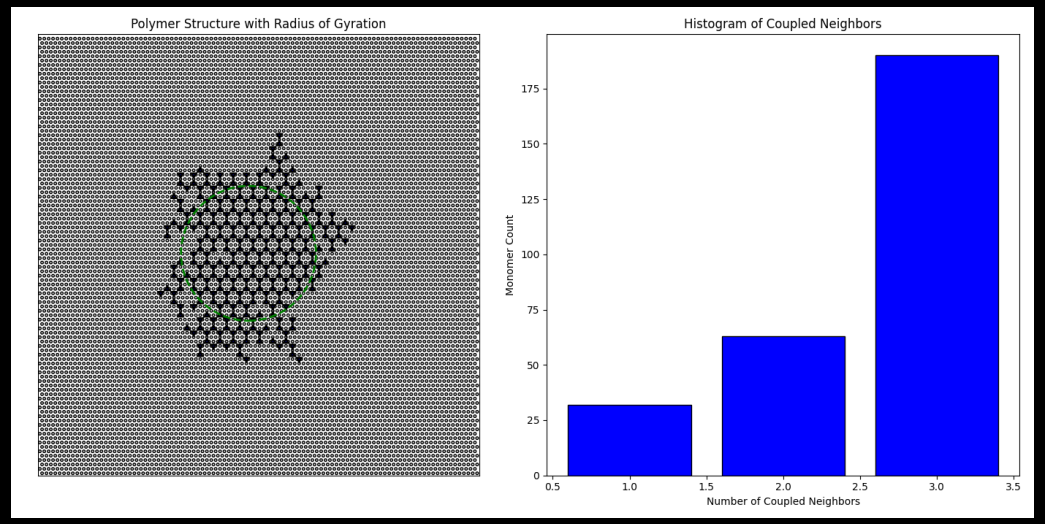
Results

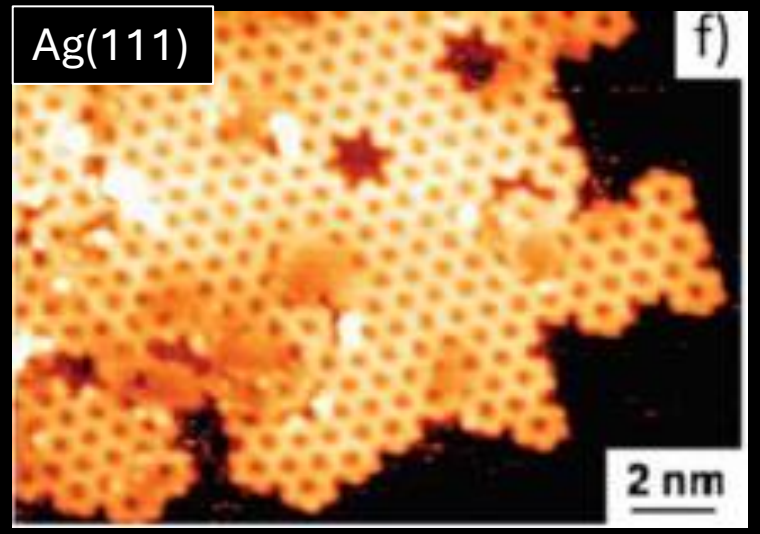
High diffusion barrier, low coupling barrier





High coupling barrier, low diffusion barrier





Bieri, et al. *JACS* **2010** *132* (46)

Next Steps

- Introduce surface defects, like step edges, point defects, etc.
- Model **copolymerization**, where two different monomer species can polymerize together as **block-**, or as **random-copolymers**
- Scale up the model to analyze how islands merge