Engineering Novel Self-Assembling Peptide Materials via Simulations of Diphenylalanine

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Engineering New Nanoscale Materials From Peptides

- Self-assembling peptide materials
  - Form variety of nanostructures
  - Cheap, easy to make
  - Environmentally benign
  - Easily manipulated using known biochemistry

- Diphenylalanine nanotubes
  - Stable
  - Strong
  - Unique properties

Reches and Gazit. Science. 2003
Applications of Diphenylalanine Nanotubes

• Grow discrete Ag nanowires

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• Increase electrode surface area and performance in supercapacitors

Simulating Self-Assembly at a Molecular Level

- Driving forces for self-assembly
- Reasons for stability
- Mechanism/pathway of self-assembly
All-Atom Simulations

- Explicitly represent every atom and their physical interactions
- Limited to small-scale systems
Analyzing Crystal Structure Stability

- Contact map
  - Counts number of times atoms are close to each other in simulation
  - Measures relative strength of interactions
Twelve Free Peptides in a Box of Water

- Stronger electrostatics
- Second ring interactions still prevalent
Similarities with Crystal Structure Increase with Concentration
Results and Conclusions

• Crystal structure stabilized principally by aromatic and hydrophobic interactions

• Early self-assembly driven by amphiphilicity

• Similarities with crystal structure increase with concentration
Future Work

• Simulate larger systems

• Simulate vacuum conditions

• Identify novel variants of diphenylalanine with increased stability for experimental testing

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