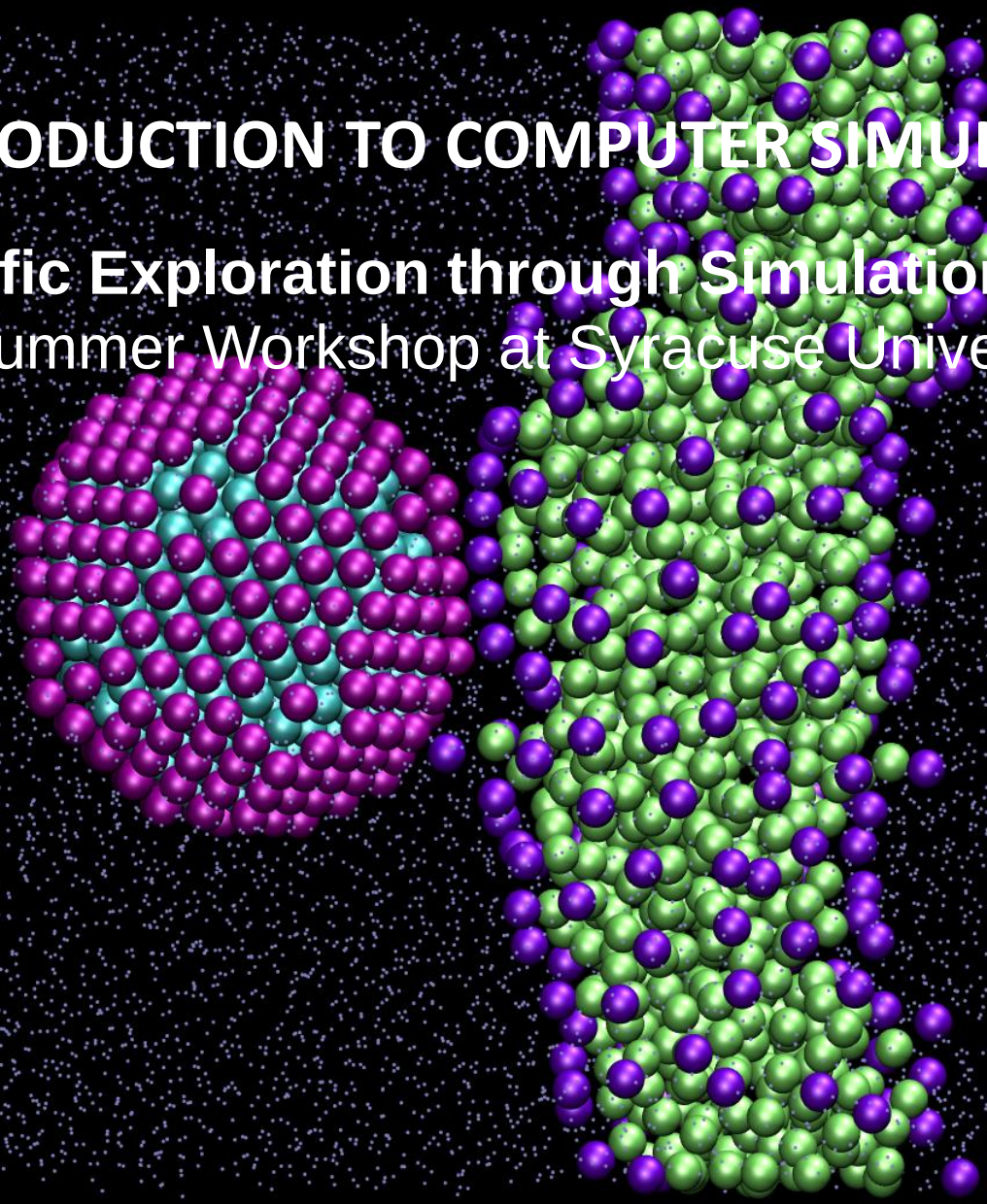
INTRODUCTION TO COMPUTER SIMULATIONS

Scientific Exploration through Simulations (SETS)

Summer Workshop at Syracuse University



COMPUTER SIMULATIONS

- "A **computer simulation**, a **computer model**, or a **computational model** is a computer program, or network of computers, that attempts to simulate an abstract model of a particular system."
  http://en.wikipedia.org/wiki/Computer_simulation

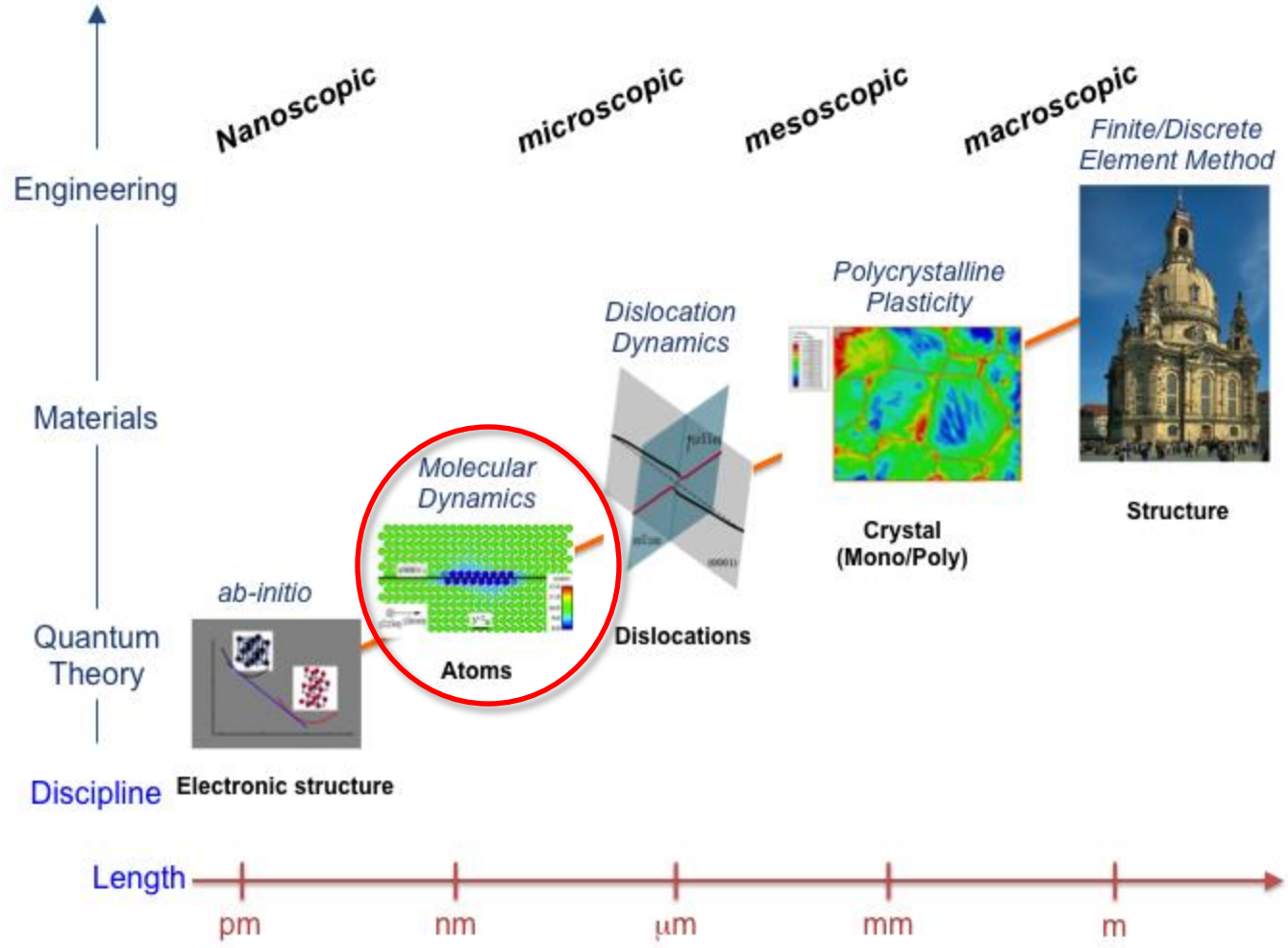
- Simulations are used in the fields of physics, chemistry, biology, engineering, economics, finance, political sciences and meteorology among others with one or many of the objectives below.
  - Hypothesis Testing
    - More on hypothesis:
      http://examples.yourdictionary.com/examples/examples-of-hypothesis.html
  - Hypothesis Generation
  - Prediction
  - Understanding/visualizing of phenomena inaccessible to experiments
  - Design
  - Optimization

Discussion: provide examples for the use of computer simulations in the above contexts.

ELEMENTS OF A COMPUTER SIMULATION

- **Motivation—e.g. scientific curiosity to better understand a physical system, technological applications, etc.**
- **A Sound Model—a set of rules/constraints or mathematical equations that govern the structure, movement and properties of the system at hand**
- **Algorithm—a systematic, faithful and efficient way to "solve" the model equations**
- **Fast Computers—10s to 100s of processors in house, 1000s on central facilities (e.g. Blue Gene at Brookhaven National Lab.)**
  - **SU's Green Data Center: https://www.syr.edu/greendatacenter/index.html**
  - **New York Blue at Brookhaven National Laboratory http://www.bnl.gov/newyorkblue/**
- **Archival, Analysis and Interpretation of Data**
- **Comparison with Experimental Observations and Known Results**
- **Summary of Key Findings and Recommendations (including how one might improve the simulation itself)**

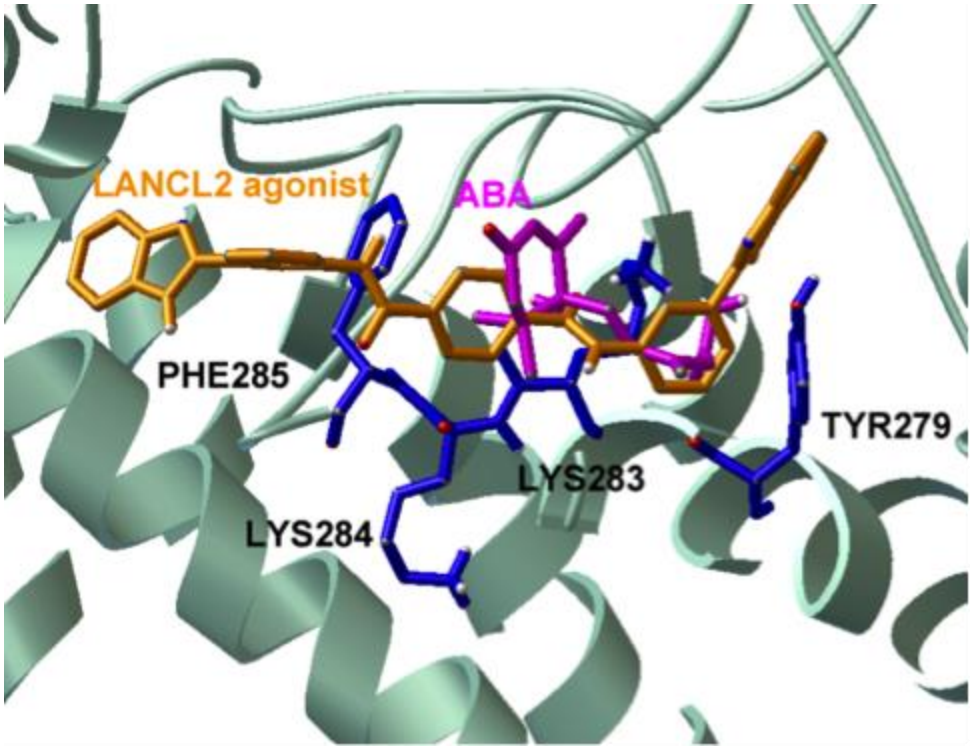
COMPUTER SIMULATIONS: PICO- TO MACRO-SCALES
e.g. Materials Science & Engineering



http://tu-freiberg.de/fakult4/imfd/cms/Multiscale/Multiscale.png

MOLECULAR SIMULATIONS: EXAMPLES

DRUG DESIGN

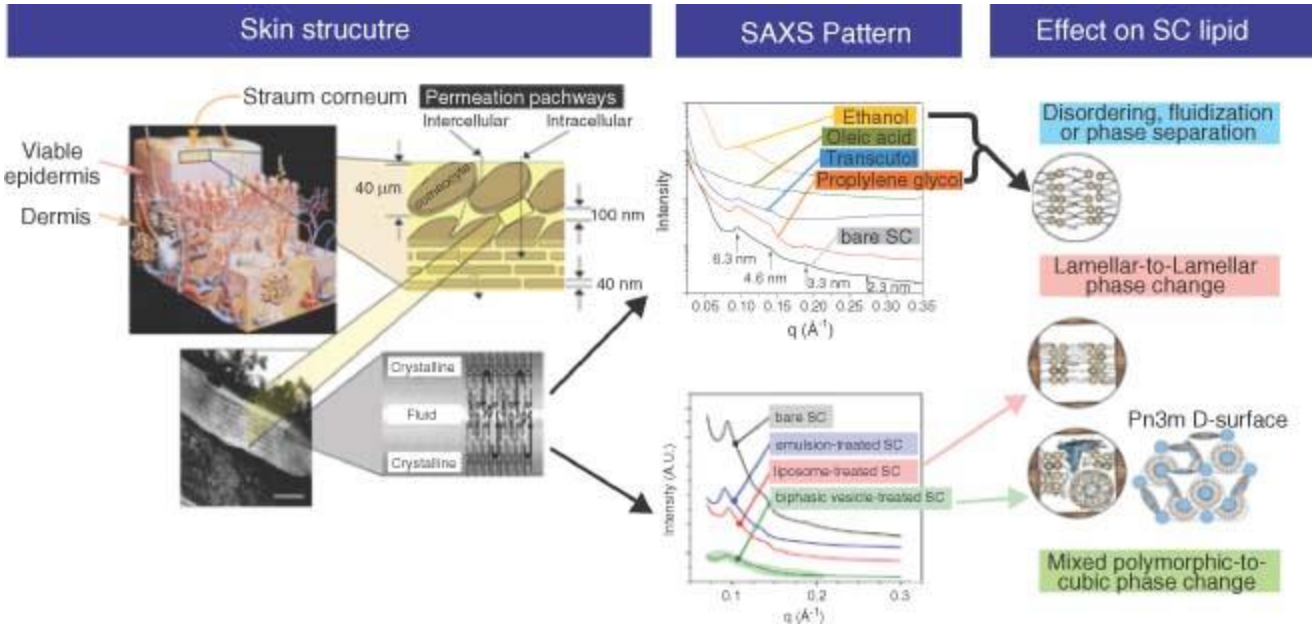


Molecular dynamics are most often used to predict the conformation of a small molecule (drug) and to model conformational changes in the biological target that may occur when the small molecule binds to it.

http://www.nimml.org/technologies/bioinformatics-and-hpc/computer-aided-drug-design/

MOLECULAR SIMULATIONS: EXAMPLES

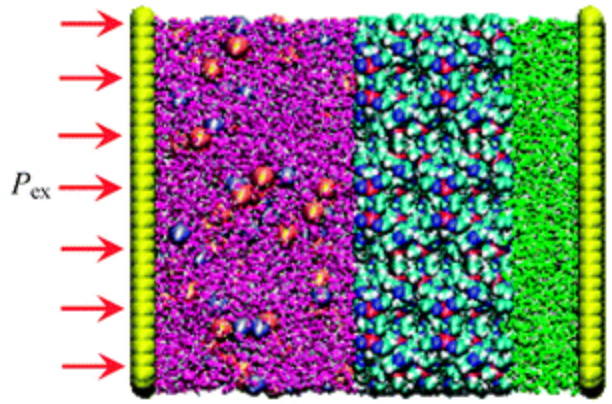
DRUG DELIVERY



From: "Drug delivery through the skin: molecular simulations of barrier lipids to design more effective noninvasive dermal and transdermal delivery systems for small molecules, biologics, and cosmetics"
http://wires.wiley.com/WileyCDA/WiresArticle/wisId-WNAN147.html

MOLECULAR SIMULATIONS: EXAMPLES

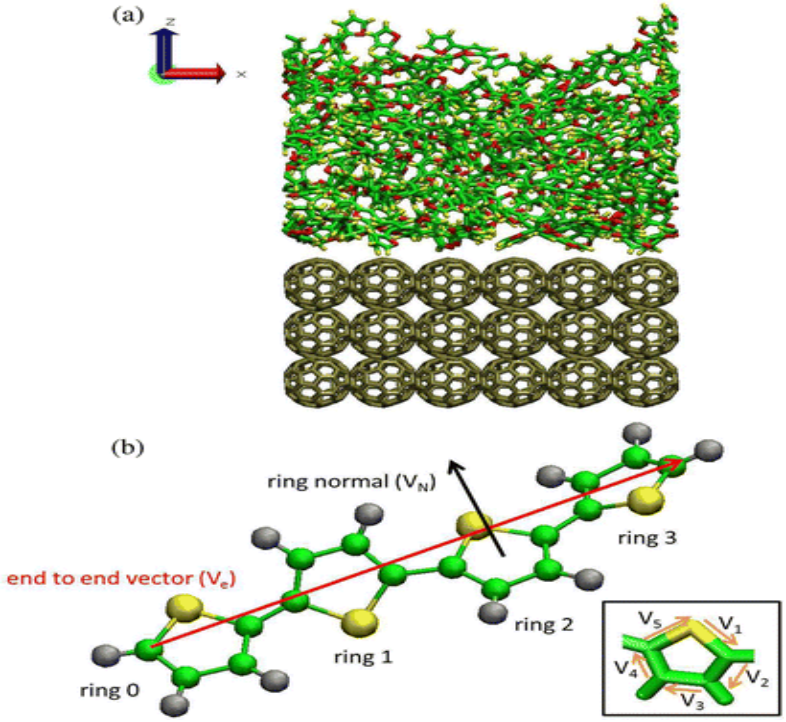
WATER DESALINATION



Water desalination through a nano (ZIF-8) membrane. Two chambers are separated by the ZIF-8 membrane: the one on the left is 0.5 M NaCl aqueous solution and the other on the right is pure water bath. An external pressure is exerted on the left chamber to mimic a reverse osmosis process.
http://pubs.rsc.org/en/content/articlehtml/2011/cs/c0cs00128g

MOLECULAR SIMULATIONS: EXAMPLES

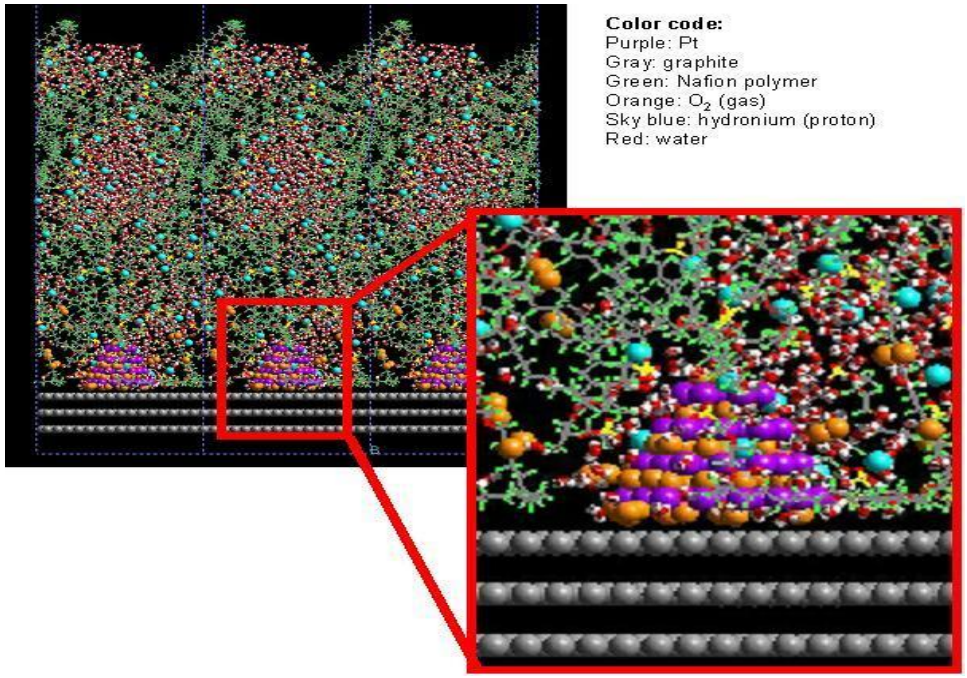
ORAGANIC PHOTOVOLTAICS (SOLAR CELLS)



Snapshot of simulation box used to investigate OPV materials. Fullerene molecules are shown in dark green, on top of which oligothiophene molecules are adsorbed. (b) Snapshot of a single oligothiophene molecule in detail, showing the four rings for each molecule. The sulfur atoms are colored yellow, carbons are green, and hydrogens are gray. http://pubs.acs.org/doi/full/10.1021/jp212548r

MOLECULAR SIMULATIONS: EXAMPLES

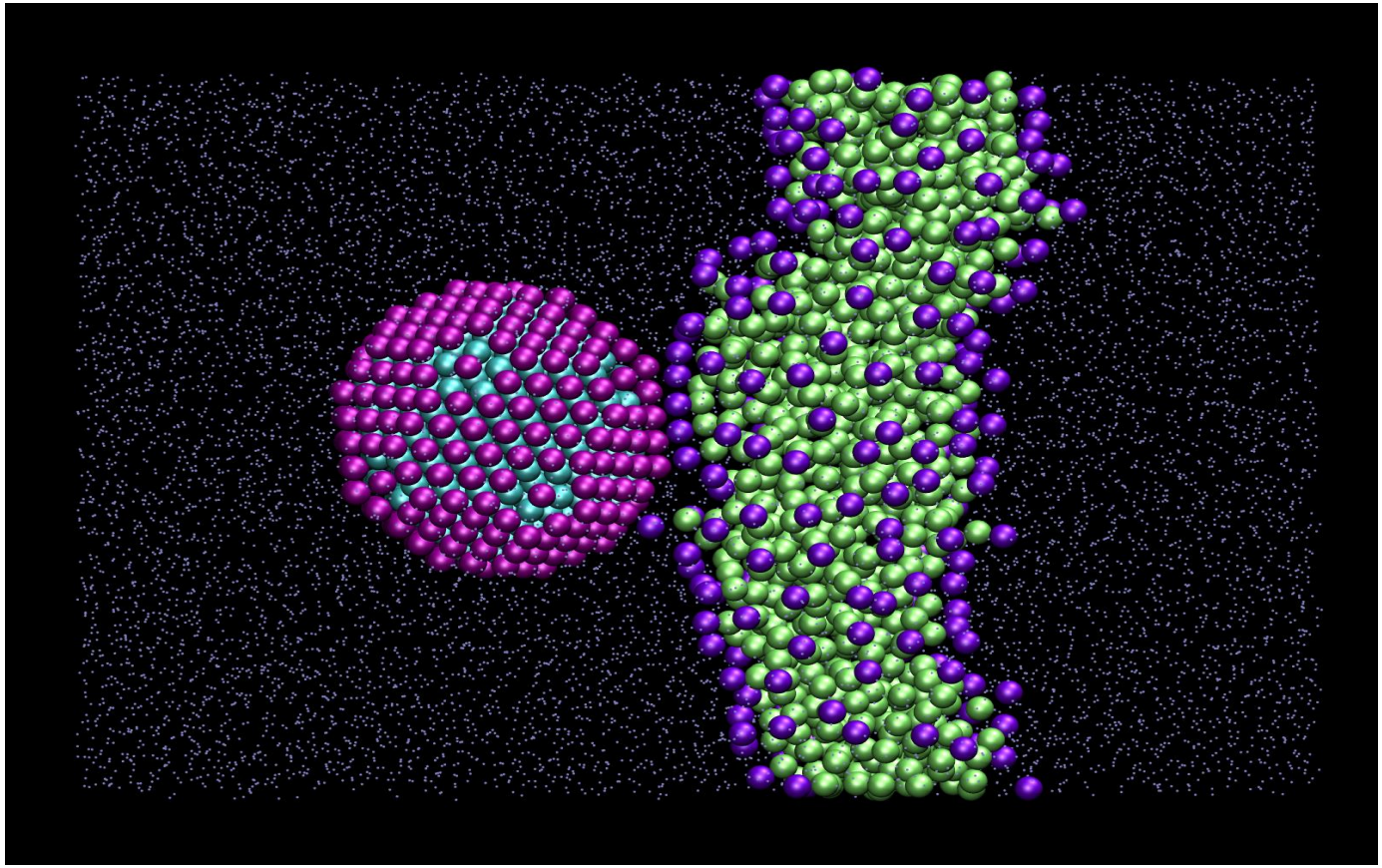
FUEL CELLS



Model for simulating the Platinum/Nafion Interface in a Polyelectrolyte Membrane Fuel Cell. http://www.wag.caltech.edu/fuelcells/projects/Nafion.html

MOLECULAR SIMULATIONS: EXAMPLES

NANOTECHNOLOGY



Molecular dynamics simulation setup to probe the interactions between a nanoparticle and a polymer strand in aqueous solution. The system size is 15 nm.
A. Sambasivam & R. Sureshkumar (2012)

MOLECULAR SIMULATIONS: Further Examples

Each participant identifies an application of molecular simulations (use Google search).