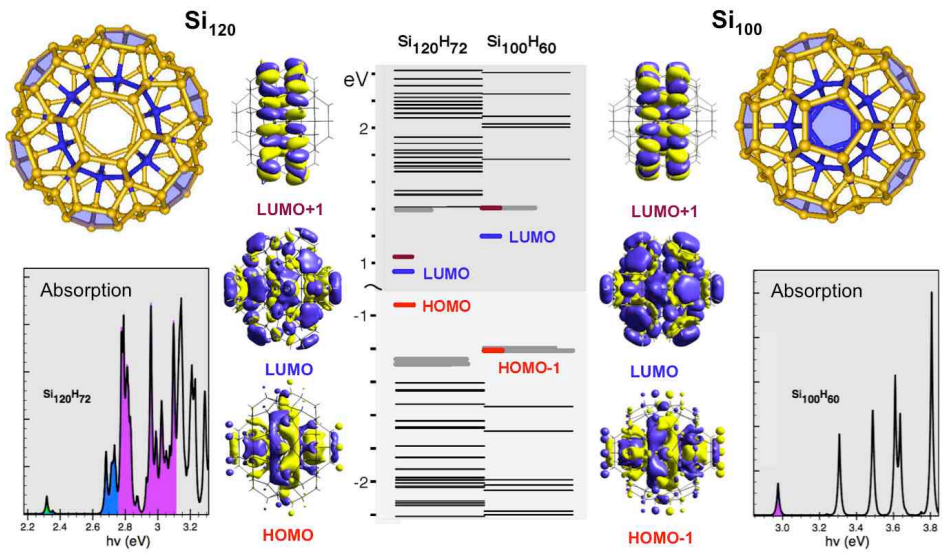
# Molecular Dynamics Simulations of Time-Dependent and Transport Processes

Traian Dumitrica, Department of Mechanical Engineering, University of Minnesota

• This project develops a molecular dynamics code and applies it to describe the microscopic response of nano-objects to nonequilibrium electronic distributions. The code developing part was accomplished.

• We have also performed a preliminary study on the thermodynamic stability and optical properties of Si dots and nanowires. One important finding is that the dot's shape can be used to control optical properties. In highly symmetric dots, even small shape changes can dramatically affect the optical response (see figure). The shape modulation (intrinsic or under strain) can prove interesting for gap engineering and for tuning the optical absorption.




Two Si dots of the same size have different optical properties.

## Current Work

• With the new code, we are now performing simulations to explore the potential of laser pulses to induce transformations at the nanoscale, and to study the structural stability of current-carrying nanostructures.