AE 714

Atomistic modeling of materials

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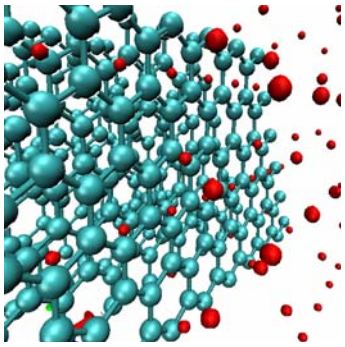

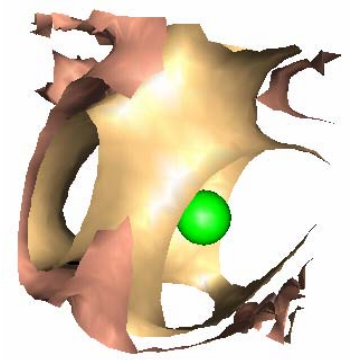

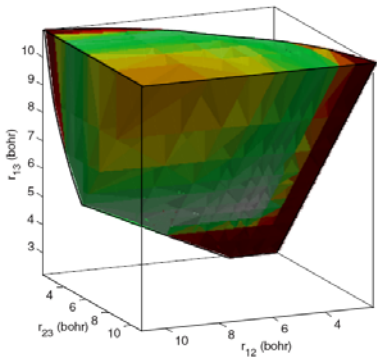

Catalog description: The new course is intended for engineering graduate students with interests in the simulation of materials at the atomic scale using academic and commercial software. Specific topics include: Monte Carlo and molecular dynamics simulations, density functional theory and the total-energy pseudopotential method, free energy and phase transitions, linear response theory, rare event simulations, first-principles molecular dynamics and dynamical Monte Carlo models. The course includes lectures covering theoretical aspects followed by computational lab sessions at the CAEN Windows training rooms (Duderstadt center) where students will be trained in atomistic simulations.

Maximum class size is restricted to 25 students so that each student gets individual access to a CAEN machine.

Intended audience: Graduate Students in Engineering with interests in materials, nanotechnologies and modeling at the atomic/electronic scale.