MSEN5377 - Computational Physics of Nanomaterials

MSEN 5377 (PHYS 5377) Computational Physics of Nanomaterials (3 semester hours) This course introduces atomistic and quantum simulation methods and their applications to modeling study nanomaterials (nanoparticles, nanowires, and thin films). The course has three main parts: basic theory of materials (thermodynamics, statistical mechanics, and solid state physics), computational methods to model materials systems, and applications to practical problems. There are three main themes of the course: structure-property relationship of nanomaterials; atomistic modeling for atomic structure optimization; and quantum simulations for electronic structure study and functional property analysis. Prerequisite: MSEN 6319 or equivalent. (3-0) R