
MM 13: HV Yip

Time: Tuesday 9:30–10:00

Location: H16

Invited Talk

MM 13.1 Tue 9:30 H16

Computational Materials — ●SIDNEY YIP — Department of Nuclear Science and Engineering and Materials Science and Engineering, Massachusetts Institute of Technology, Cambridge, MA 02139-4307 (USA)

Computational science – the use of advanced computing capabilities to solve complex problems – has become critical to all scientific and technological endeavors in our society, whether it is for scientific leadership as in universities, for economic competitiveness in corporate research laboratories, or for national security in government agencies. At the intersection of computational science and materials research is a sweetspot for the physics community, offering fundamental challenges

as well as technologically relevant applications. This talk will examine the role of multiscale modeling and simulation in providing insights to mechanical and thermal behavior of condensed matter, with a view towards materials characterization and design. A central theme is shear stability and localization which manifest in considerations of theoretical strength of crystals, thermodynamic versus mechanical melting, solid-state amorphization, and brittle to ductile transition in fracture. Another theme is thermal and electron transport in a class of problems which combine chemical physics with materials science. These investigations pave the way to tackling even more complex phenomena in materials the technological significance of which is quite transparent, such as viscous flow of molten glass, hardening kinetics of cement paste, and deformation of tempered steel in fatigue.