The Ben May Center for Chemical Theory and Computation



Modeling Materials: Continuum, Atomistic and Multiscale Concepts and Techniques

At a Glance

WHAT Condensed two-week e-course (Sunday-Thursday + Sunday-Thursday, 15:00-19:00 each) on the fundamentals of continuum, atomistic and multiscale modeling of materials.

WHO Prof. Ellad B. Tadmor (U. Minnesota, USA) and **Prof. Ronald E. Miller** (Carleton University, Canada).

WHERE Zoom

WHEN August 16-27, 2020 15:00-19:00 each day

ACADEMIC 2 credit points will be given to CREDIT Physics and Chemistry students

About the Course

Material properties emerge from phenomena on scales ranging from angstroms to millimeters, and only a multiscale treatment can provide a complete understanding. Materials researchers must therefore understand fundamental concepts and Quasicontinuum simulation of techniques from vastly different fields.



interaction of crack and grain boundary.

This e-course is an intensive 2-week introduction to the fundamentals required to understand stateof- the-art modeling and computer simulation of material behavior. The course includes a mix of theoretical lectures, exercises, and hands-on practical computer calculations. The following topics will be covered:

• Continuum mechanics: tensors, nonlinear deformation, balance laws, thermodynamics, constitutive relations, energy principles.

- Finite Element Method (FEM): nonlinear FEM, basic theory, practical simulations.
- Materials Science: crystals and defects.
- Quantum mechanics: basic theory, density functional theory, tight binding.
- Classical atomistic modeling: interatomic potentials, statistical mechanics, molecular dynamics (MD), stress and heat flux in MD.
- Spatial multiscale methods: Cauchy-Born rule, static and dynamic atomistic/continuum coupling methods, Quasicontinuum method.

Participants will receive copies of the textbooks "Modeling Materials" (Tadmor and Miller) and "Continuum Mechanics and Thermodynamics (Tadmor, Miller and Elliott) published by Cambridge University Press, 2012.

About the Instructors

Professors Tadmor and Miller have been teaching and researching the science of multiscale materials modeling for 20 years. Between them, they have published over 120 scientific articles and two books. They have received numerous awards for both their research and teaching abilities.

Who Can Attend

This course is open to Physics, Chemistry and Math students (MSc and PhD) and postdocs (though only Physics and Chemistry students will be given academic credit). No prior knowledge is assumed

Additional details and Registration

The complete e-course details are available at the FGS online course system, see this link (Course 20201172)

Weizmann students should register through the FGS online course system. Weizmann postdocs and non-Weizmann students can apply by sending an e-mail to: Terry Debesh terry.debesh@weizmann.ac.il

Commitment

All accepted participants commit themselves to attend the whole course, with no exception, and to provide feedback on the course