ΕΙΧΗΜΥΘ-ΙΤΕ

ΣΕΜΙΝΑΡΙΟ

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ΘΕΜΑ: Multiscale modelling of materials properties

ΤΟΠΟΣ: Αίθουσα Σεμιναρίων ΕΙΧΗΜΥΘ - ΙΤΕ

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ΠΕΡΙΛΗΨΗ

Large deformations of solids under external loading defy a simple description based on constitutive laws due to possible phase transformations and the presence of strain way beyond the elastic limit. Chemical reactions in the high-stress environment near a loaded crack tip present an additional complication to the response of the solid and are related to phenomena like corrosion and embrittlement. In these cases, a quantum mechanical approach for simulating electronic behavior is indispensable, as chemical bonds are being broken or rearranged under unusual conditions. However, not all the bonds in an inhomogeneously strained system are subjected to the same amount of distortion; in regions where the distortion of chemical bonds from their equilibrium is small, empirical methods, which are also computationally more efficient, suffice. Combining methodologies that can describe with adequate accuracy the different regions in solids is a challenge to computational modelling. We will discuss recent advances in developing such methodologies and their applications to realistic systems. The applications include intentation of silicon, a prototypical brittle material, the switching mechanism in a pieozoelectric as a function of strain and external electric field, and the simulation of crack behavior in a chemically active environment under external load.