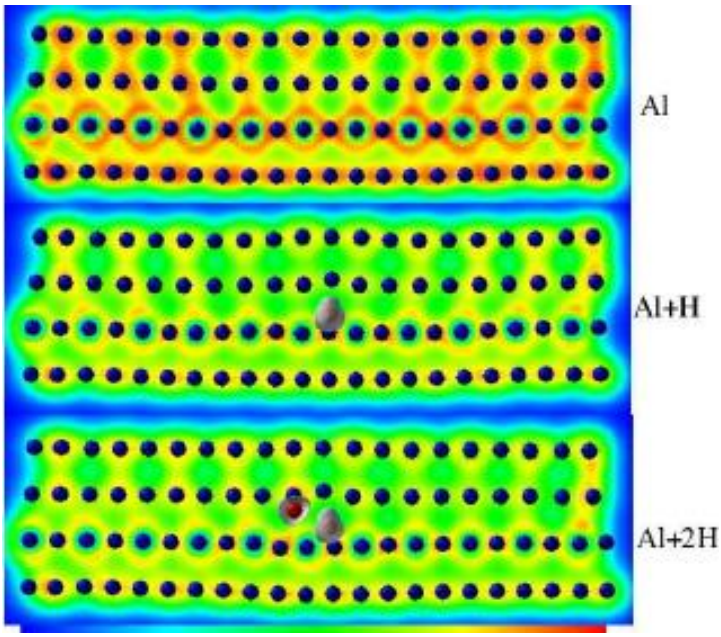
COLLOQUIUM



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Quantum Simulations of Materials Behaviors at Large Scale: from Finite Elements to Electrons by QCDFT Method

Abstract

The fracture mechanism is a fundamental and critical issue for designing advanced materials and systems with enhanced safety margin and energy efficiency. A typical fracture in a solid material always starts with electronic bonds breaking at the scale of angstroms (10^{-10} m), spanning several orders of magnitude in scale of space. It is desired to have electrons modeled in large scale modeling of materials mechanical properties when electronic bonds breaking and forming are involved. Quasi-Continuum Density Functional Theory (QCDFT) method is a full scale modeling of materials from finite elements to electrons based *entirely* on quantum mechanics. All energies and forces are calculated from first-principles density functional theory without any empirical parameters. In this talk, the QCDFT method will be introduced, emphasizing on the quantum mechanical/finite element coupling. Examples of QCDFT applications in hydrogen embrittlement in metals will be discussed.

2:00-3:00 p.m., Friday, May 11th, McLane Hall 162
Special time. All are welcome!