

1036-82-85

Emily A Carter* (eac@princeton.edu), Department of Mechanical and Aerospace Engr,
Program in Applied and Computational Math, Princeton University, Princeton, NJ 08544.

Quantum-Based Multiscale and Multiphysics Simulations of Materials.

Our goal is to develop an honest, rigorous, and accurate mathematical and computational description of complex solid materials. Unfortunately, no single universal theory exists that accomplishes this objective. Because of the complexity of features and interactions across length scales and material type, one must resort to a heterogeneous coupling of theories, in which the physics of each phenomena or feature is well described. We also wish to avoid the conventional engineering approach of fitting to experimental data, and prefer to start from the basic laws of physics that describe materials, namely quantum mechanics, so as to have an independent source of data for comparison to experiment. In our present work, we start with solid state density functional theory to describe the quantum nature of electrons and then couple the resulting information with various statistical mechanical approaches (e.g. molecular dynamics, kinetic Monte Carlo, rare event theory), as well as, with solid mechanics continuum methods, to get a much more detailed picture of how materials behave. We will discuss salient aspects of our approach, validity tests, and predictions of the behavior of metals subjected to stress and/or corrosive elements. (Received January 15, 2008)