Electronic structure calculations at macroscopic scales

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Defects play a crucial role in influencing the macroscopic properties of solids—examples include the role of dislocations in plastic deformation, dopants in semiconductor properties, and domain walls in ferroelectric properties. These defects are present in very small concentrations (few parts per million), yet, produce a significant macroscopic effect on the materials behavior through the long-ranged elastic and electrostatic fields they generate. The strength and nature of these fields, as well as other critical aspects of the defect-core are all determined by the electronic structure of the material at the quantum-mechanical length-scale. Hence, there is a wide range of *interacting* length-scales, from *electronic structure to continuum*, that need to be resolved to accurately describe defects in materials and their influence on the macroscopic properties of materials. This has remained a significant challenge in multi-scale modeling, and a solution to this problem holds the key for *predictive* modeling of complex materials systems.

In an attempt to address the aforementioned challenge, this talk presents the development of a *seamless* multi-scale scheme to perform electronic structure calculations at macroscopic scales. The key ideas involved in its development are (i) a real-space variational formulation of electronic structure theories, (ii) a nested finite-element discretization of the formulation, and (iii) a systematic means of adaptive coarse-graining retaining full resolution where necessary, and coarsening elsewhere with no patches, assumptions or structure. This multi-scale scheme has enabled, for the first time, calculations of the electronic structure of multi-million atom systems using orbital-free density-functional theory, thus, paving the way for an accurate electronic structure study of defects in materials. The accuracy of the method and the physical insights it offers into the behavior of defects in materials is highlighted through studies on vacancies and dislocations. Current efforts towards extending this multi-scale method to Kohn-Sham density functional theory will also be presented.