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Electronic structure calculations at macroscopic scales using orbital-free DFT[1] BALACHANDRAN GADAGUNTLA RADHAKRISHNAN, VIKRAM GAVINI, University of Michigan — Defects play a crucial role in influencing a wide range of material properties and their energetics are determined by the electronic-structure of the core of a defect as well as long-ranged elastic and electrostatic effects. In this work, we present the development of a seamless multi-scale method that enables electronic structure calculations on multi-million atom systems using orbital-free DFT. The key ideas that constitute the method are: (i) a local real-space variational formulation of orbital-free DFT including the recently proposed kernel energies for kinetic energy functionals; (ii) an adaptive coarse-graining of the finite-element basis, which is used to discretize the formulation, retaining full resolution where necessary and coarse-graining elsewhere. We demonstrate the accuracy and effectiveness of the method through studies on mono-vacancy and di-vacancies in aluminum. Our results show remarkable cell-size effects in the energetics of vacancies, and suggest much larger computational domains than those considered previously are necessary in electronic-structure studies on defects.

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