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**Quasi-continuum orbital-free density-functional theory (QC-OFDFT)** VIKRAM GAVINI, KAUSHIK BHATTACHARYA, MICHAEL ORTIZ, California Institute of Technology — Density-functional theory has provided insights into various materials properties in the recent decade. However, its computational complexity has made other aspects, especially those involving defects, beyond reach. Here, we present a seamless coarse-graining scheme for orbital-free density-functional theory (OFDFT), that enables the study of multi-million atom clusters with no spurious physics and at no significant loss of accuracy. The key ideas are (i) a real-space formulation, (ii) a nested finite-element implementation 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. Fully-resolved OFDFT and finite lattice-elasticity are obtained as special limits of this scheme. This methodological development has enabled OFDFT calculations on large systems, which have revealed interesting physics and phenomena that have not been observed to date.

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