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Nonorthogonal generalized hybrid Wannier functions for linear scaling DFT simulations of surfaces and interfaces ANDREA GRECO, ARASH MOSTOFI, Imperial College London, JOHN FREELAND, Argonne National Laboratory — Semiconductor-based thin-films have applications in microelectronics, from transistors to nano-capacitors. Many of their properties depend on phenomena at multiple length scales, but their complexity makes it difficult to obtain a detailed understanding of their behavior from experiment alone. First-principles simulations based on density-functional theory (DFT) are invaluable for providing insight into materials' properties including for the study of thin films. In particular, hybrid Wannier functions (WFs), fully extended in the surface plane, but localized along the direction normal to the surface, have been successfully used to explore the properties of systems layered along a given direction. The large length scales associated with structures and processes in more realistic surfaces, however, are beyond the scope of such calculations, because they rely on first performing a traditional cubic-scaling DFT calculation. To overcome this limitation we extend the concept of hybrid WFs to nonorthogonal orbitals that are directly optimized in situ in the electronic structure calculation. We show that this method, implemented in the ONETEP linear scaling DFT code, enables the study of large-scale surfaces and interfaces with plane-wave accuracy but at reduced computational expense.

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