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Nonorthogonal generalized hybrid Wannier functions for large-scale DFT simulations[1] ANDREA GRECO, Imperial College London, JOHN W. FREELAND, Argonne National Laboratory, ARASH A. MOSTOFI, Imperial College London — Semiconductor-based thin-films have applications in microelectronics,from transistors to nanocapacitors. Many properties of such devices strongly depend on the details of the interface between a metallic electrode and the thin-film semiconductor/insulator. Hybrid Wannier Functions (WFs), extended in the surface plane, but localized along the direction normal to the surface/interface, have been successfully used to explore the properties of such heterostructures layered along a given direction, and are a natural way to study systems that are at the same time a 2D conductor (in plane) and a 1D insulator (out of plane). Current state-of-the art implementations of Hybrid WFs rely on first performing a traditional cubic-scaling density-functional theory (DFT) calculation. This unfavourable scaling precludes the applicability of this method to the large length scales typically associated with processes in realistic structures. 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 implement this method in the ONETEP large-scale DFT code and we apply it to realistic heterostructure systems, showing it is able to provide plane-wave accuracy but at reduced computational cost.

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