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A new Laplacian representation for real-space calculations of general periodic and partially periodic systems AMIR NATAN, AYELET BENJAMINI, DORON NAVEH, LEEOR KRONIK, Weizmann Inst of Sci, MURILO TIAGO, SCOTT BECKMAN, JAMES CHELIKOWSKY, University of Texas, WEIZMANN INST OF SCI TEAM, UNIVERSITY OF TEXAS TEAM — We present a real-space method for electronic-structure calculations of systems with general full or partial periodicity. The method is based on the self-consistent solution of the Kohn-Sham equations, using first principles pseudopotentials, on a uniform three-dimensional non-Cartesian grid. Its efficacy derives from the introduction of a new generalized high-order finite-difference Laplacian that avoids the numerical evaluation of mixed derivative terms and results in a simple yet accurate finite difference operator. Our method is further extended to systems where periodicity is enforced only along some directions (e.g., surfaces), by setting up the correct electrostatic boundary conditions and by properly accounting for the ion-electron and ion-ion interactions. Our method enjoys the main advantages of real-space grid techniques over traditional plane-wave representations for density functional calculations, namely, improved scaling and easier implementation on parallel computers, as well as inherent immunity to spurious interactions brought about by artificial periodicity. We demonstrate its capabilities on bulk GaAs and Na for the fully periodic case and for a monolayer of Si-adsorbed polar nitrobenzene molecules for the partially periodic case.

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