

Abstract Submitted
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Optimized basis sets for coarse-grained electronic structure calculations of point defects BJÖRN LANGE, CHRISTOPH FREYSOLDT, JÖRG NEUGEBAUER, MPIE Düsseldorf — Density-functional theory is a powerful tool to study the properties of point defects in the supercell approach. Yet, the size limitations make a description of the extended tails of defect states, especially for shallow defects, cumbersome. Atomic orbital basis sets are the method of choice to coarse-grain electronic structure calculations, but are in general not flexible enough for describing the unusual bonding situations, which occur in point defects. We employ a newly developed method that, based on a variational principle, allows to generate small atomic basis sets which optimally mimic the Kohn-Sham wavefunctions with a plane-wave basis set. We show that these basis sets accurately reproduce the underlying plane-wave calculation. We analyze how the atomic orbitals close to the defect are modified in comparison to their bulk counterparts. We are able to extend basis sets generated from small supercells and to reproduce the bandstructure of larger cells. Using this approach we construct and solve a reliable sparse model Hamiltonian for a shallow defect test system containing $10^3..10^4$ atoms.

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