Abstract Submitted
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Bloch-state-based interpolation – an efficient generalization of the Shirley approach to interpolating electronic structure[1] DAVID PRENDERGAST, The Molecular Foundry, Lawrence Berkeley National Laboratory, STEVEN G. LOUIE, Dept. of Physics, University of California Berkeley and The Molecular Foundry, LBNL — We present an efficient generalization of the k-space interpolation scheme for electronic structure presented by E. L. Shirley, Phys. Rev. B **54**, 16464 (1996), which permits the construction of a compact k-dependent Hamiltonian using a numerically optimal basis derived from a coarse-grained set of density functional theory calculations. We provide some generalizations of the initial approach which reduce the number of required initial electronic structure calculations, enabling accurate interpolation over the entire Brillouin zone based on calculations at the zone-center only for large systems. We also generalize the representation of non-local Hamiltonians, leading to a more efficient implementation which permits the use of both norm-conserving and ultrasoft pseudopotentials in the input calculations. Numerically interpolated electronic eigenvalues with accuracy that is within 0.01 eV can be produced at very little computational cost. The approach is also applicable to other theoretical frameworks such as the Dyson equation for quasiparticle excitations or the Bethe-Salpeter equation for optical responses.

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