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Shirley Reduced Basis DFT: plane-wave generality and accuracy at reduced computational cost[1] MAXWELL HUTCHINSON, University of Chicago, DAVID PRENDERGAST, The Molecular Foundry, Lawrence Berkeley National Laboratory — The Shirley Reduced Basis (SRB) provides a means for performing density functional theory electronic structure calculations with plane-wave accuracy and generality in a basis of significantly reduced size. The SRB is comprised of linear combinations of periodic Bloch functions sampled coarsely over the Brillouin zone (BZ) and selected for maximal information content using proper orthogonal decomposition [E. Shirley, Phys. Rev. B 54, 464 (1996)]. A basis produced from only order 10 samples, lying on the BZ boundary, is able to reproduce energies and stresses to sub meV and kbar accuracy, respectively, with order 10 basis functions per electronic band. Unlike other electronic structure bases of similar sizes, the SRB is adaptive and automatic, making no model assumptions beyond the use of pseudopotentials. We provide the first self-consistent implementation of this approach, enabling both relaxations and molecular dynamics. We demonstrate the usefulness of the method on a variety of physical systems, from crystalline solids to reduced dimensional systems under periodic boundary conditions, realizing order of magnitude performance improvements while kept within physically relevant error tolerances.

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Maxwell Hutchinson
University of Chicago

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