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Finding Symmetry-adapted Wannier Functions from L_1 Sparse Optimization JIATONG CHEN, Department of Materials Science and Engineering, University of California, Los Angeles, KE YIN, Department of Mathematics, University of California, Los Angeles, YI XIA, VIDVUDS OZOLINS, Department of Materials Science and Engineering, University of California, Los Angeles, STANLEY OSHER, RUSSEL CAFLISCH, Department of Mathematics, University of California, Los Angeles — Wannier functions have applications in numerous fields of condensed matter physics, from polarization and orbital magnetization to topological insulators and linear-scaling methods for electronic structure calculations. We present a technique to calculate symmetry-adapted Wannier functions that are strictly localized within a finite region based on the framework of compressed Wannier modes [V. Ozolins, R. Lai, R. Caflisch, S. Osher. Proc. Natl. Acad. Sci. USA 2014 111 (5) 1691-1696]. Our method does not require a prior computation of the band structure, but directly minimizes a functional that is the sum of the total energy and an L_1 regularization term $\frac{1}{\mu}\int |\psi| d\mathbf{r}$, which drives strict localization. One parameter μ controls the trade-off between the localization and the energy accuracy. Here we show how symmetry constraints can be incorporated in this formalism, leading to Wannier functions that form irreducible representations of the crystal group. Since only $\mathbf{k}$ points from the irreducible wedge of the Brillouin zone need to be considered, the computational effort is similar to that required for conventional band structure calculations.

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