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Symmetry-adapted Wannier Functions from L_1 regularized Sparse Optimization JIATONG CHEN, KE YIN, YI XIA, VIDVUDS OZOLINS, STANLEY OSHER, RUSSEL CAFLISCH, Univ of California - Los Angeles — Wannier functions are widely used as real space representation of periodic solids in electronic structure calculation. We present a new approach to calculate symmetry-adapted Wannier functions which are directly obtained from variational principle of total energy plus an L1 regularization term, $\frac{1}{\mu}\int |\psi| d\mathbf{r}$. The obtained compressed Wannier functions are only nonzero within a finite region. With the help of induced group representation theory, we only need to calculate Bloch functions (in Wannier gauge) within irreducible Brillouin zone, while point group symmetry is strictly enforced. Implementation in plane waves-pseudopotential codes and application to real material system will be demonstrated.

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