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Constructing Wannier functions with automatically selected trial orbitals¹ JAMAL I. MUSTAFA, SINISA COH, MARVIN L. COHEN, STEVEN G. LOUIE, University of California at Berkeley, Lawrence Berkeley National Lab — Maximally localized Wannier functions (MLWFs) are widely used in electronic structure theory. Some applications include analysis of chemical bonding, electric polarization, orbital magnetization, and Wannier interpolation. The state of the art method for constructing MLWFs of N composite bands is based on the method of Marzari and Vanderbilt (MV)² and is implemented in the Wannier90 code. One of the practical difficulties in constructing Wannier functions using the MV method is choosing N trial orbitals with roughly the same angular character and location as the target N Wannier functions. We avoid this practical difficulty with a new scheme, by starting from a large set (M , larger than N) of lowest lying atomic orbitals and then selecting an optimal subspace of N trial orbitals as a starting point. We investigate this approach on silicon structures of varying complexity, as well as the topological insulator Bi_2Se_3 where construction of Wannier functions for occupied electronic states is especially hard.

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²Marzari, N., and D. Vanderbilt Phys. Rev. B 56, 12847 (1997).

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