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Selectively Localized and Symmetric Wannier Functions RUNZHI WANG, Columbia Univ, EMANUEL LAZAR, University of Pennsylvania, HYOWON PARK, ANDREW MILLIS, CHRIS MARIANETTI, Columbia Univ — The method of Marzari and Vanderbilt for computing maximally localized Wannier functions (MLWF) is widely used to represent localized orbitals in periodic materials. However the standard MLWF method minimizes the global spread of all orbitals in a preselected energy window. In many methods for strongly correlated electronic systems, including the density functional plus dynamical mean field method, one wishes to localize one particular class of orbitals (ie. a transition metal d orbital) without regard for the localization of the other states (eg. oxygen p and s). In addition, guaranteed preservation of pre-specficied point symmetry is desirable. Here we present an approach to this problem and demonstrate its implementation in model systems and real materials.

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