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Selectively localized Wannier functions RUNZHI WANG, Columbia University, EMANUEL LAZAR, University of Pennsylvania, HYOWON PARK, University of Illinois at Chicago, ANDREW MILLIS, CHRIS MARIANETTI, Columbia University — Since the seminal work of Marzari and Vanderbilt, maximally localized Wannier functions have become widely used as real-space representations of electronic structure in periodic systems. In this talk we discuss selectively localized Wannier functions (SLWF) which allow localization of a particular subset of orbitals of interest, and also enable the fixing of orbital centers and ensuring the preservation of point-group symmetries. Applications of our method to GaAs, $SrMnO_3$, and Co demonstrate that SLWF can offer improvements over standard techniques, especially in beyond DFT methods.

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