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Generalized optimization of Wannier functions EMANUEL LAZAR, HYOWON PARK, CHRIS MARIANETTI, ANDY MILLIS, Columbia University —
Marzari and Vanderbilt introduced and developed a technique for defining and computing "maximally localized" Wannier functions to represent localized orbitals in periodic materials [1]. Since then, this method has been heavily used in computational condensed matter physics calculations. The Marzari-Vanderbilt procedure localizes all orbitals in a given energy window. In this talk we present some ongoing work in generalized minimization strategies which can apply different constraints to different subspaces of the manifold (for example, localizing some orbitals more than others). Applications to model systems and more realistic low-dimensional materials are presented.

[1] Marzari et al. Rev. Mod. Phys. 84, 1419 (2012).

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