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Unfolding first-principles band structures[1] WEI KU, T. BERLIJN, Brookhaven National Laboratory; Stony Brook University, C.-C. LEE, Brookhaven National Laboratory — A general method [1] is presented to unfold band structures of first-principles supercell calculations with proper spectral weight, allowing easier visualization of the electronic structure and the degree of broken translational symmetry. The resulting unfolded band structures contain additional rich information from the Kohn-Sham orbitals, and absorb the structure factor that makes them ideal for a direct comparison with angle resolved photoemission spectroscopy experiments. With negligible computational expense via the use of Wannier functions, this simple method has great practical value in the studies of a wide range of materials containing impurities, vacancies, lattice distortions, or spontaneous long-range orders.

[1] Wei Ku, T. Berlijn, and C.-C. Lee, Phys. Rev. Lett. **104**, 216401 (2010).

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