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Wannier Center Sheets in Topological Insulators[1] MARYAM TAHERINEJAD, KEVIN GARRITY, DAVID VANDERBILT, Rutgers University
— The electronic ground state in a periodic crystalline insulator can be described by hybrid Wannier functions $|W_{nl_z}(k_x, k_y)\rangle$ which are maximally localized in one direction and Bloch-like in the other two. In 3D insulators the Wannier charge centers (WCCs), defined as $\bar{z}_n(k_x, k_y) = \langle W_{n0}(k_x, k_y)|\hat{z}|W_{n0}(k_x, k_y)\rangle$, are functions of momentum in two dimensions and can be plotted as sheets over the 2D Brillouin zone. We show that the symmetry group of the WCCs $\bar{z}_n(k_x, k_y)$ includes all the symmetries of surface energy bands $\epsilon_n(k_x, k_y)$. More importantly, the WCCs contain the same kind of topological information as is carried in the surface energy bands, with the crucial advantage that the topological properties of the bulk can be deduced from bulk properties alone. The distinct topological behavior of these WCC sheets in trivial, Chern, weak, strong, and crystalline topological insulators are demonstrated using different tight-binding models. The WCC sheets calculated from first-principles calculations in Z_2-even Sb_2Se_3, weak Z_2-odd KHgSb, and strong Z_2-odd Bi_2Se_3 confirm the results from the tight-binding models.

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