Three-Dimensional Multi-Orbital Flat Band Models and Materials

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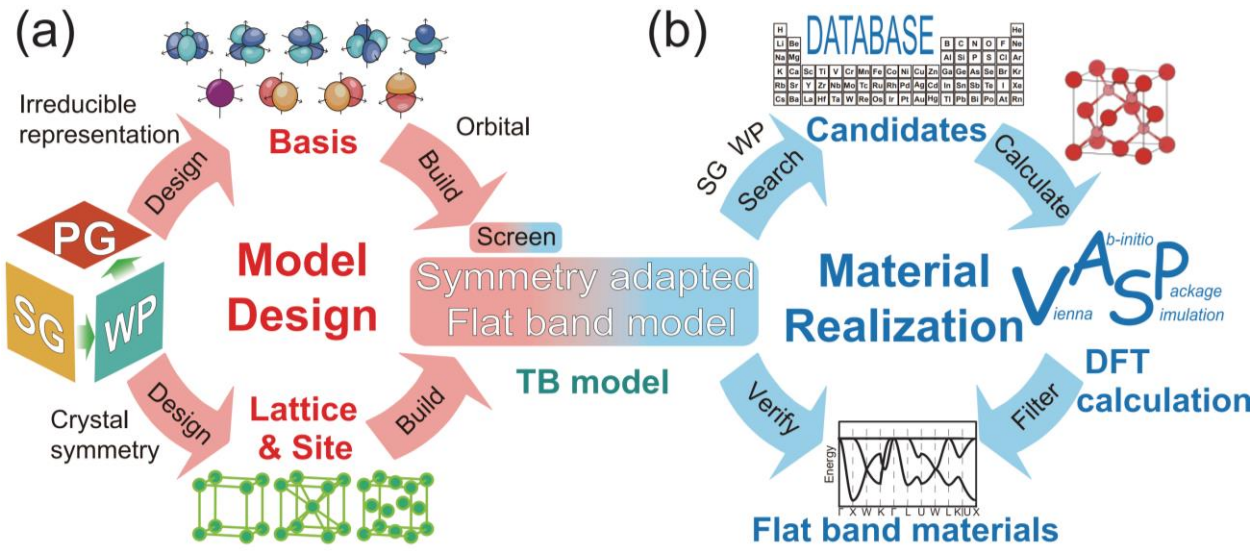
The study of flat band (FB) models and their physical manifestations serve as a crucial basis for probing exotic quantum phenomena associated with strong correlation. Here we present a systematic theoretical framework that simultaneously enable the construction of multi-orbital FB models and identification of feasible material candidates. This is achieved by integrating group theory and crystallography for the symmetry-adapted tight-binding model, which incorporate lattice, site, and orbital degrees of freedom. We elucidate this framework's practical applicability by uncovering a novel three-dimensional (3D) multi-orbital FB model in the basic face-centered cubic lattice, fundamentally distinct from typically studied single-orbital Lieb and Kagome models. Most importantly, we successfully identify a plethora of high-quality binary material candidates exhibiting ultra-clean 3D FB near the Fermi level. We further show the diversity of orbital bases within the model and expand our analysis to other cubic lattices with varying space groups for the realization of various 3D multi-orbital FB systems. We believe that this research lays a solid foundation for studying the correlated physics of FB systems, especially for multi-orbital systems.



Pic. 1 *Theoretical framework for exploring multi-orbital FB systems.* The FB searching framework contains two modules. (a) The first module handles the FB model design based on symmetry-adapted TB model designing, building, and screening processes, which consider the lattice, site, and orbital degrees of freedom. SG, PG, and WP represent the space group, point group, and Wyckoff position, respectively. (b) The second module handles the material realization by treating the FB materials searching, calculating, filtering and verification processes. It searches material candidates using the WP and SG information from the model design process, followed by high-throughput DFT calculations, and FB material verification.