Symmetry-Respecting Wannier Functions and Their Applications in Strongly Correlated Materials: New Development of First-Principles Many-Body Down-Folding Approach

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Based on a flexible first-principles construction of symmetry-respecting Wannier functions, a novel many-body down-folding approach is recently developed to derive the low-energy effective Hamiltonian that governs the physics of strongly correlated materials. In this talk, representative applications of these Wannier functions will be surveyed, including studies of ferromagnetism in half-filled cuprates [1], gapless charge density wave in dichalcogenides [2], charge/orbital order in manganites [3,4], and charge excitations in the oxides [5,6]. As an illustration of the new many-body down-folding method, detail discussions will focus on the recent discovery of the super-repulsion effect in the high-Tc cuprates and its significant implications [7].

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