Electronic-structure studies of low-dimensional nanomaterials

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First-principles electronic structure calculations offer powerful tools for understanding the properties of quantum materials and interpreting experimental results. In this talk, I will introduce the basic concepts of electronic structure calculations and discuss our computational studies of various low-dimensional nanomaterials. From iron-based superconductors to moiré materials and nanostructures, first-principles density functional theory (DFT) and its advanced extensions are utilized to investigate quantum-mechanical properties such as strong electron correlation, electron-phonon interaction, and nonequilibrium quantum transport. For each system, I will emphasize the relevance of our calculations to experimental findings.