

Ab-initio Green's functions methods for molecules and solids.

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This talk will address current theoretical challenges in modeling solid-state materials and summarize recent advances made by my group in developing *ab-initio* methods for solids. In the first part, a relativistic, self-consistent GW approach for weakly correlated materials will be presented. Based on the exact two-component formalism, this method enables the accurate treatment of scalar relativistic effects, spin–orbit coupling, and the interplay between relativistic phenomena and electron correlation without adjustable parameters.

The second part will focus on strongly correlated electrons in the d- and f-shells of transition-metal compounds. Embedding techniques that allow these electrons to be treated without a significant increase in computational cost will be discussed. Illustrative results will be shown for correlation effects in SrMnO_3 and BiVO_3 , as well as Néel temperatures in NiO , MnO , and CoO . The talk will conclude with an outlook on promising directions for future research.