Modeling Complex Materials: A NMTO-Wannier Function Approach

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Muffin tin orbitals (MTOs) constitute an accurate and flexible local-orbital basis set which may be chosen as minimal. This is important not only for the economy of density-functional (DFT) calculations, but also for the interpretation of results. In this talk I shall introduce NMTO method (N-th order Muffin Tine Orbital method) as an useful tool for modeling and understanding physics and chemistry of complex materials. The effectiveness of this method will be demonstrated by considering examples for correlated electron materials like high-temperature superconducting cuprates, low-dimensional quantum spin systems and the classical problem of V_2O_3.