

Wannier Functions for Strongly Correlated Systems: the Intriguing Physics of BaVS₃ as a Test Case

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An understanding of the physics of strongly correlated multi-orbital electron systems is one of the key ingredients in order to describe a wide range of novel solid state compounds. The complex interplay of the crystal structure with the competition between the localized and the itinerant character of electrons in a manifestly multi-orbital case is giving rise to highly interesting physical phenomena.

By combining the Dynamical Mean Field Theory (DMFT) with the Local Density Approximation (LDA) to Density Functional Theory, a powerful many-body approach is provided to tackle the given problem on a realistic level. This unified approach is naturally formulated by introducing Wannier(-like) functions as the basis representation for the electronic structure problem [1,2,3]. The choice of Wannier functions is not unique in various senses and has to be tailored to the physical problem of interest as well as to the utilized theoretical framework.

We will discuss recent developments in this important area of interfacing realistic band-structure methods with DMFT by presenting results for the complex BaVS₃ compound. In the latter system, electronic correlations are relevant in driving orbital charge transfers and Fermi-surface deformations in the metallic regime [3,4,5]. The paramagnetic insulating charge-density wave state shows moreover a complex orbital structure with important differences between the V ions [5].

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