

Direct Generation of Wannier Functions by Downfolding, Polynomial Approximation, and Symmetrical Orthonormalization

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Localized, minimal basis sets are useful for numerous purposes in electronic-structure calculations. Such a basis may pick a single band or a complex of bands, say the occupied bands, and may uncover the bonding, enable real-space order- N calculations, provide understanding, or be used to construct low-energy Hubbard Hamiltonians for correlated systems. We shall explain how to generate such basis sets directly by Löwdin downfolding (partitioning) from a large, complete, basis set of energy-independent, highly localized orbitals such as AOs or LMTOs, and subsequent removal of the energy dependence of the downfolded orbitals by the N -ization technique [1,2]. When applied to energy-dependent partial waves, rather than AOs or LMTOs, this gives rise to the NMTO method [3-6]. An orbital of the minimal basis set is simply the original orbital, dressed by a cloud of those orbitals which have been removed from the original set by downfolding. If the minimal basis set is chosen to span particular bands, symmetrical orthonormalization yields a set of localized Wannier functions. Wannier functions which are maximally localized in some other sense may be obtained by a subsequent unitary transformation for a local cluster [1,2]. For most correlated d - and f -electron systems, no further localization is achieved by the last step [1,2,7]. Examples from NMTO calculations will be presented [8-12].

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