**NMTO Wannier-like functions for insulators and metals**

**Part I**

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**Introduction:**

Wannier functions can be a very powerful tool in the study of solids. In particular, they provide an understanding of the chemical bonding of a system. Moreover, they can be used as an accurate minimal basis in order-N methods and to construct effective Hamiltonians for studies of, for example, strongly correlated systems. In this poster, we describe the features of NMTO (Muffin Tin Orbitals of order N) Wannier-like functions. We will in particular show that they can be used for gaining a chemical understanding of the electronic structure of insulating and metallic systems.

**Graphite: π-bonding and anti-bonding bands**

Downfolding within multiple-scattering theory, followed by formation of NMTOs lead to a truly-minimal basis set, which describes a group of bands, a band, or merely the occupied part of a band.

The NMTO basis set, \( \chi^{(N)}(r) \), for a given energy mesh, \( \varepsilon_0, \varepsilon_1, \ldots, \varepsilon_N \), spans the solutions, \( \psi_j(k;r) \), of Schrödinger's equation for the overlapping MT-potential, \( V(r) = \sum_R V_R^N(r-R) \), with errors

\[
\delta\psi_j(k;r) \propto [\varepsilon_j(k) - \varepsilon_0] [\varepsilon_j(k) - \varepsilon_1] - [\varepsilon_j(k) - \varepsilon_N].
\]

For an isolated set of bands, the truly minimal NMTO basis converges as the energy mesh spans the range of the band and gets finer and finer. Orthonormalization of the converged NMTO set therefore yields a set of Wannier functions. These are localized, because the NMTOs are localized by construction: E.g., an orbital of the \( \sigma_p \)-set spanning the \( \sigma \)-bands is confined by the condition that it has no \( \sigma_p \)-character on the other carbon atoms. All other characters are downfolded, i.e., they are whatever is appropriate for the energy mesh; they are passive.

In all figures, the black bands have been calculated using a full basis set, while the red ones have been calculated using the specified minimal basis. The energy mesh, \( \varepsilon_0, \varepsilon_1, \ldots, \varepsilon_N \), employed is given to the right of the band structure. Note: In all figures, the black bands have been calculated using a full basis set, while the red ones have been calculated using the specified minimal basis. The energy mesh, \( \varepsilon_0, \varepsilon_1, \ldots, \varepsilon_N \), employed is given to the right of the band structure.

**Graphite: \( \sigma \)-bonding bands**

In order to describe the \( \sigma \)-bonding bands in graphite, put an \( \sigma_p \) and \( \sigma_p \) NMTO on every second carbon atom, and downfold all other channels.

**Boron Nitride: \( \pi \) - and \( \sigma \)-bonding bands**

In the above, we have seen that for an insulator, and even a semi metal, we can design an NMTO basis set which describes only the occupied bands. It is therefore natural to associate an orbital with a pair of electrons. With atom-centered orbitals we would then use the extreme ionic limit: in boron nitride, we would use a \( B^5N^4 \) basis set. However, the NMTO method is forgiving even the \( B^5N^4 \) basis works. However, for the \( \pi \)-bands we need more energy points to describe the bands properly.