Band selection and disentanglement using maximally-localized Wannier functions: the cases of Co impurities in bulk copper and the Cu (111) surface

Richard Korytár[1], Miguel Pruneda[1], Javier Junquera[2], Pablo Ordejón[1], Nicolás Lorente[1]

[1] *Centro de investigación en nanociencia y nanotecnología (CSIC - ICN), Campus de la UAB, E-08193 Bellaterra, Spain*

[2] *Departamento de ciencias de la Tierra y física de la materia condensada, Universidad de Cantabría, E-39005 Santander, Spain*

rkorytar@cin2.es

We have adapted the maximally-localized Wannier function approach of [1] to the density functional theory based `Siesta` method[2] and applied it to the study of Co substitutional impurities in bulk copper as well as to the Cu (111) surface. In the Co impurity case, we have reduced the problem to the Co d-electrons and the Cu sp-band, permitting us to obtain an Anderson-like Hamiltonian from well defined density functional parameters in a fully orthonormal basis set. An important insight into the impurity problem is provided by the projected density of states onto the impurity Wannier functions (Fig. 1), showing sharp spin and crystal field polarized peaks. This confirms the picture of a localized state weakly perturbed by the continuum.

In order to test the quality of the Wannier approach to surfaces, we have studied the electronic structure of the Cu (111) surface by again transforming the density functional problem into the Wannier one. This can be in turn diagonalized (Fig. 2), showing that an excellent description of the Shockley surface state is attained, permitting us to be confident in the application of this method to the study of magnetic adsorbates in the presence of an extended surface state.

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[1] I. Souza, N. Marzari, and D. Vanderbilt, Phys. Rev. B **65**, 035109 (2001).

[2] J. M. Soler et al., Journal of Physics: Condensed Matter **14**, 2745 (2002).

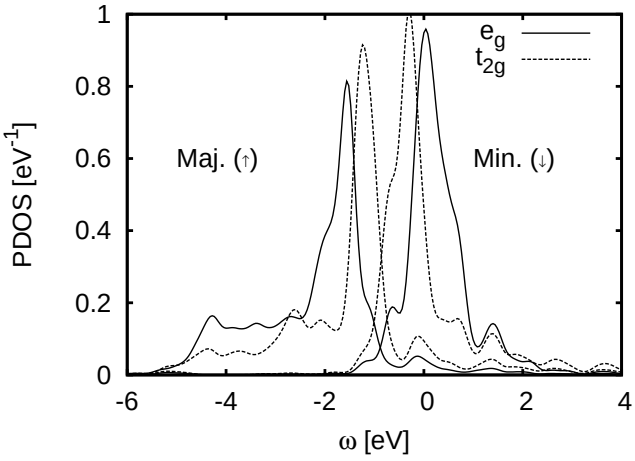

FIG. 1: Cobalt Wannier-function projected density of states for both spins. Zero energy coincides with Fermi level.

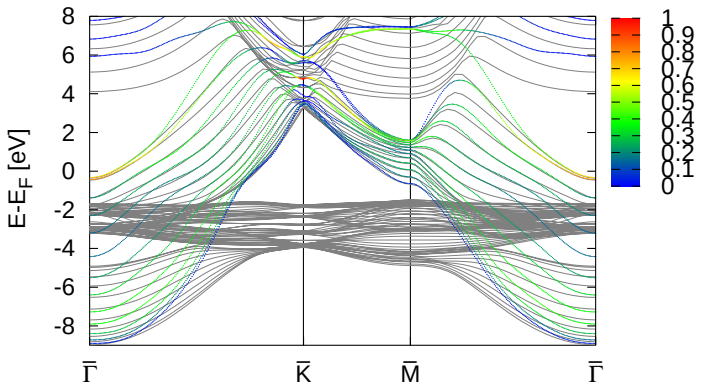

FIG. 2: Comparison of ab-initio band structure (grey) with the Wannier (color) of a Cu (111) slab. Color indicates the admixture of surface Wannier functions to the eigenstate.