Maximally Localized Wannier Functions: Ultrasoft Pseudopotentials and Related Applications

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The use of maximally localized Wannier functions (MLWFs) recently became very popular in the electronic structure community, as a supplementary analysis tool. On one hand, MLWFs are attractive because they constitute a localized basis set which is complete and orthonormal, while on the other hand, they also carry physical information. Is it therefore a direct interest of the community to improve and generalize the current methods and algorithms to compute MLWFs.
In the framework of the WanT [1] project, we developed and implemented [2] a theoretical scheme that enables the calculation of maximally localized Wannier functions in the formalism of projector-augmented-waves [3] and ultrasoft-pseudopotentials [4]. I will describe this formalism as well as some technical issues related to the computation of MLWFs. I will also discuss some application of the above method to the calculation of spontaneous polarization and surface dipole for SiC polytypes, and to the evalutation of transport properties in organic-silicon interfaces.

[1] WanT project, `http://www.wannier-transport.org`.

[2] A. Ferretti, A. Calzolari, B. Bonferroni, and R. Di Felice, J. Phys.: Condens. Matt. **19**, 036215 (2007).

[3] P. E. Blöchl, Phys. Rev. B **50**, 17953 (1994).

[4] D. Vanderbilt, Phys. Rev. B **41**, R7892 (1990).