The electronic-structure genome of inorganic materials

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Abstract

Maximally localized Wannier functions (MLWFs) are widely used in condensed matter physics and computational materials science. However, the construction of MLWFs used to rely on chemical intuition, constituting a roadblock for many researchers. Here, we showcase the automated algorithms and robust workflows we have developed to tackle such issues, addressing the cases of both metals and insulators [1,2]. On top of these, we build several MLWF databases for over 20,000 3D inorganic crystals and 2000 exfoliable 2D monolayers. These databases represent an "electronic-structure genome", as minimal but exact compressed encoding of the electronic structure of each material. Moreover, they provide accurate calculations of many materials properties, thanks to the very efficient Wannier interpolations. We demonstrate the power of the setup with three applications in materials discovery: (a) high-performance thermoelectrics, (b) topological materials with large nonlinear Hall effect, and (c) heterostructures with polar discontinuity for two-dimensional electron gases. We will also discuss how to reach beyond-DFT accuracy in the prediction of electronic-structure excitations (e.g., charged excitations such as band structures) using Koopmans spectral functionals [3,4].

References

[1] J. Qiao, G. Pizzi, and N. Marzari, npj Comp. Mat., 9 (2023) 208.
[2] J. Qiao, G. Pizzi, and N. Marzari, npj Comp. Mat., 9 (2023) 206.
[3] https://koopmans-functionals.org/en/latest/references.html
[4] E. B. Linscott, N. Colonna, R. De Gennaro, N. L. Nguyen, G. Borghi, A. Ferretti, I. Dabo, and N. Marzari, J. Chem. Theor. Comput. 19 (2023) 7097.

Figures

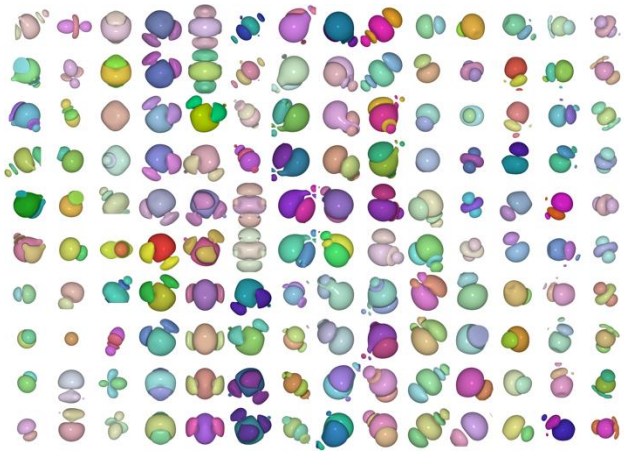

Figure 1. Isosurfaces for some of the 1.3M+ MLWFs obtained.