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Building a beyond-DFT database of spectral functions for correlated materials[1] SUBHASISH MANDAL, KRISTJAN HAULE, KARIN RABE, DAVID VANDERBILT , Rutgers University — Generating databases of the electronic structure of materials is a key to data-science-driven materials discovery. Many existing materials databases, which were constructed in the spirit of the Materials Genome Initiative, rely almost exclusively upon DFT engines and often make incorrect predictions for many correlated materials. Because qualitative predictions of excited-state properties usually require beyond-DFT methods, various advance methods such as meta-GGAs, hybrid functionals, GW, and dynamical mean-field theory (DMFT) have been developed to describe the electronic structure of correlated materials. However, the expected accuracy of these methods when applied to various classes of materials remains unclear. It is thus of pressing interest to compare their accuracy for different types of materials, and at the same time, to build a broad publicly-available database of the results of beyond-DFT calculations[1]. In this talk, I will discuss some of the challenges involved in generating such a beyond-DFT database, and show how we have overcome these challenges in our systematic study of these methods on various training sets of moderately and strongly correlated materials. [1]https://jarvis.nist.gov/jarvisbdft/;Mandal et al. npj. Comput. Mater. 5, 115 (2019); arXiv:2101.03262

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