Reproducibility in density functional theory calculations of solids

The success and widespread popularity of density-functional theory (DFT) over the last decades has given rise to an extensive range of dedicated codes for predicting molecular and crystalline properties. However, each code implements the formalism in a different way, raising questions about the reproducibility of such predictions. In this article, the results of a community-wide effort is reported, comparing 15 solid-state codes, using 40 different potentials or basis set types, to assess the quality of the equations of state for 71 elemental crystals. The overall conclusion is that predictions from recent codes and pseudopotentials agree very well, with pairwise differences that are comparable to those between different high-precision experiments. Results of older methods, however, show stronger discrepancies.

exciting, the program package [1,2] developed in the group of Claudia Draxl at the Humboldt-Universität zu Berlin (Physics Department and **IRIS Adlershof**) represents one of the all-electron full-potential implementations of DFT. It employs the linearized-augmented planewave basis, which is considered the gold standard within the condensed-matter community. Within this study, **exciting** has proven to be among the three most precise packages, with nearly negligible differences between them.

exciting has not only evolved into a benckmark code for DFT but has a strong focus on excitations that are treated within time-dependent DFT and many-body perturbation theory. In August 2016, *HoW exciting! 2016* [3] will take place at the Campus Adlershof, consisting of an international workshop on excitations in solids and a hands-on course employing **exciting.**

[1] exciting-code.org

[2] **exciting: a full-potential all-electron package implementing density-functional theory and many-body perturbation theory**
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[3] how-exciting-2016.physik.hu-berlin.de

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