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The ground state elemental crystals as a benchmark set for solid state DFT: intrinsic accuracy and code comparison

K. Lejaeghere[1], V. Van Speybroeck[1], G. Van Oost[3], S. Cottenier[1,2]

[1] *Center for Molecular Modeling and QCMM Alliance Ghent-Brussels, Ghent University, Technologiepark 903, BE-9052 Zwijnaarde, Belgium*
[2] *Department of Materials Science and Engineering, Ghent University, Technologiepark 903, BE-9052 Zwijnaarde, Belgium*
[3] *Department of Applied Physics, Ghent University, Sint-Pietersnieuwstraat 41 B4 9000 Ghent, Belgium*

A central issue when applying DFT for property predictions is an assessment of the error bars on the computed quantities. For this purpose, a large and diverse test set for crystalline solids is presented, containing all ground state elemental crystals (except most lanthanides). The deviation between DFT-predictions and experiments are analysed for several structural properties. Trends in the deviations are discussed, and a statistically justified error bar is given to quantify the predictive quality of a DFT-result. Moreover the agreement between different codes is evaluated as well. A quality factor D is defined to quantify a generalized distance (in units of energy) between the equations of state predicted by two independent DFT packages. VASP is found to have a D-value of 2 meV with respect to WIEN2k, while for GPAW this is 4 meV.