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Test set for materials science and engineering TOKTAM MORSHEDLOO, Fritz-Haber-Institut der MPG, Berlin, DE; Ferdowsi University of Mashhad, IR, NORINA A. RICHTER, FAWZI MOHAMED, Fritz-Haber-Institut der MPG, Berlin, DE, XINGUO REN, Fritz-Haber-Institut der MPG, Berlin, DE; University of Science and Technology of China, China, SERGEY V. LEVCHENKO, LUCA M. GHIRINGHELLI, IGOR YING ZHANG, MATTHIAS SCHEFFLER, Fritz-Haber-Institut der MPG, Berlin, DE — Understanding of the applicability and limitations of electronic-structure methods needs detailed comparison with highly accurate data of representative test sets. A variety of highly valuable test sets have been established in quantum chemistry for small molecules. However, for crystalline solids they are still lacking. We present a representative test set for materials science and engineering (MSE) which includes first and second row elements and their binaries, comprising various crystal structures. This allows for unbiased benchmarking for various chemical interactions. In the MSE test set, we consider cohesive energy, lattice constant, bulk modulus, electronic, band structures and phonons etc. A big effort is made to produce systematically converged results with respect to basis set[1] and **k** mesh for a hierarchy of electronic-structure methods, ranging from the local-density approximation to advanced orbital-dependent functionals implemented in the all-electron, full-potential FHI-aims code. Furthermore, we use incremental schemes to obtain benchmark values calculated with coupled-cluster approaches.

[1] I.Y. Zhang *et al.*, *NJP* **15** 123033 (2013)

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