Supplemental material of Customizing PBE Exchange-Correlation functionals: A comprehensive approach for band gap prediction in diverse semiconductors

Satadeep Bhattacharjee,[1,*] Namitha Anna Koshi,[1] and Seung-Cheol Lee[2]

[1] *Indo-Korea Science and Technology Center (IKST), Bangalore, India*
[2] *Electronic Materials Research Center, Korea Institute of Science & Technology, Korea*

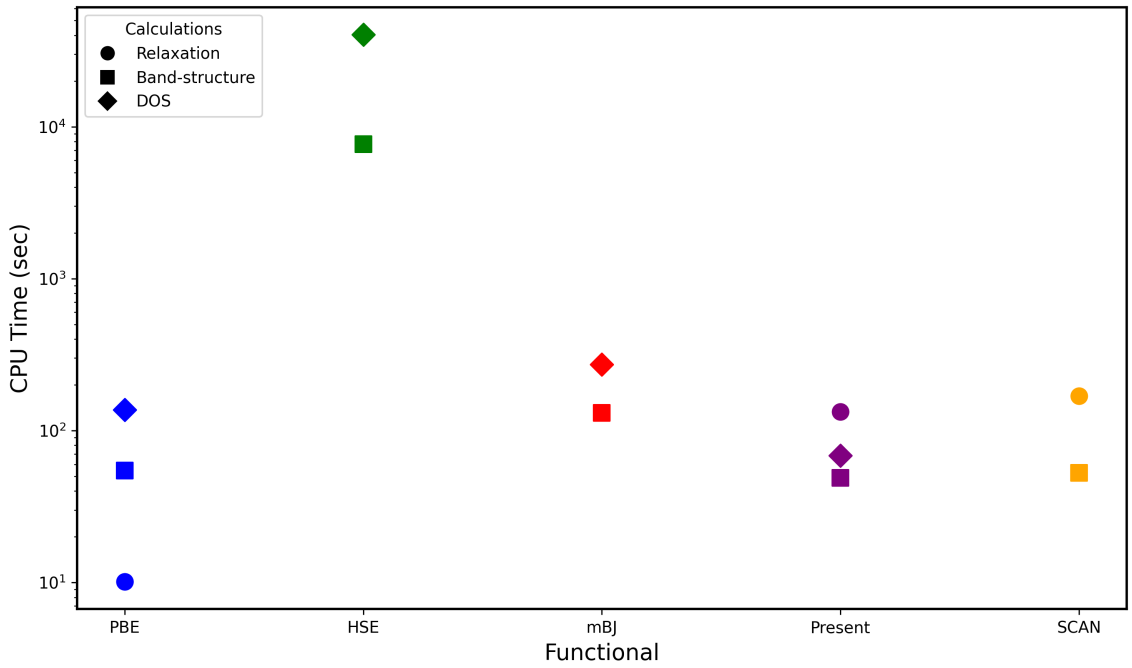

FIG. 1. Logarithmic comparison of CPU times for ZnS (Wurtzite Structure) across various functionals (PBE, HSE, mBJ, SCAN, and Present functional). The calculations include structural relaxation ("Relaxation"), band-structure ("Band-structure"), and Density of States ("DOS").

* s.bhattacharjee@ikst.res.in