

Two implementations of the Projector Augmented Wave (PAW) formalism¹

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The Projector Augmented Wave (PAW) formalism developed by Blöchl³ is an accurate and efficient pseudo-potential-like scheme for electronic structure calculations within density functional theory and is now implemented in several electronic structure codes. Some of these codes use an implementation of the formalism developed by Kresse *et al.*⁴ which differs slightly from the original Blöchl formalism and which can lead to different electronic structure results. In this poster, we analyze and illustrate the difference between the Blöchl and Kresse PAW formulations. The results of this analysis solve a long-standing mystery concerning numerical discrepancies between two independent electronic structure code packages ABINIT⁵ and PWPAW⁶. The analysis also provides insight into the development of accurate and efficient PAW basis and projector datasets.

- [1] Supported by NSF grants NSF DMR-0405456, DMR-0427055, and DMR-0705239.
- [2] In collaboration with Marc Torrent and François Jollet from CEA, DAM, DIF, F-91297 ArpaJon, France; and at WFU, summer student David Harris and graduate students Nicholas Lepley and Xiao Xu.
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