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Representability of Bloch states on Projector-augmented-wave (PAW) basis sets LUIS AGAPITO, Univ of North Texas and Duke Univ, ANDREA FERRETTI, CNR-NANO S3 Center, Istituto Nanoscienze, I-41125, Modena, Italy, STEFANO CURTAROLO, Duke University, MARCO BUONGIORNO NARDELLI, Univ of North Texas — Design of small, yet 'complete', localized basis sets is necessary for an efficient dual representation of Bloch states on both plane-wave and localized basis[1]. Such simultaneous dual representation permits the development of faster more accurate (beyond DFT) electronic-structure methods for atomistic materials (e.g. the ACBN0 method[2].) by benefiting from algorithms (real and reciprocal space) and hardware acceleration (e.g. GPUs) used in the quantum-chemistry and solid-state communities. Finding a 'complete' atomic-orbital basis (partial waves) is also a requirement in the generation of robust and transferable PAW pseudopotentials. We have employed the atomic-orbital basis from available PAW data sets, which extends through most of the periodic table, and tested the representability of Bloch states on such basis. Our results show that PAW data sets allow systematic and accurate representability of the PAW Bloch states, better than with traditional quantum-chemistry double-zeta- and double-zeta-polarized-quality basis sets.

[1]Agapito, Ferretti, Calzolari, Curtarolo and Buongiorno Nardelli, PRB **88**, 165127 (2013).
[2]Agapito, Curtarolo and Buongiorno Nardelli, `arXiv:1406.3259 [cond-mat.str-el]`

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