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PAW dataset library for the Quantum-Espresso package[1] RASHID HAMDAN, CHAO CAO, University of Florida — The frozen-core approximation is widely employed in plane-wave density functional theory calculations, because it can greatly reduce the required cut-off energy to achieve convergence. The commonly used ultra-soft pseudopotential method is one flavor of this approximation. Despite its advantages, the ultra-soft pseudopotentials are difficult to generate, and it is difficult to control the quality. It is also impossible to reconstruct the complete wave functions from the pseudopotential method calculations. The PAW method was developed to conquer these difficulties. We have constructed a set of soft, reliable PAW dataset library for the Quantum-Espresso package. The datasets were thoroughly tested, and the results were compared with VASP calculations. As a demonstration, we present the comparison with VASP calculations for Bromine doped graphite system and a comparison between the ultra-soft pseudopotential and PAW calculations of the recently discovered iron-based superconductor LaFeAsO compound. The PAW calculations yielded magnetic moment that is much closer to experimental value than the ultra-soft pseudopotential calculations.

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