From Charge Correction to Direct Modeling of Charged Systems in Plane-Wave Density Functional Theory

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Abstract

Current solutions for modeling charged systems in plane-wave density functional theory (DFT) codes such as VASP provide corrections to the unphysical behavior of an imperfect model. The imperfect model, commonly known as jellium, enforces net neutrality over the simulation cell by introducing a homogeneous background charge. These post-processing correction methods can fix a single-point calculation, however, they cannot be performed in tandem with ionic relaxations. Throughout the ionic relaxation, jellium is present and induces errors in the final geometry owing to its unrealistic nature as a mathematical artifact. Future developments into correct modeling of charged systems in plane-wave DFT will require more than a post correction of the potential and energy, self-consistent or otherwise. There is a need for a fully integrated method that models a charged system in a more physically motivated method than previous methods have attempted.[4] Here, we use contemporary methods such as Freysoldt-Neugebauer,[1] and the self-consistent potential correction[3] in a MoS_2 test system to motivate the development of a new method of modeling charged systems inside of VASP using the generalized dipole correction[2] inside the VASPsol plugin.

References

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