Local and Non-local Corrections for Charged systems in Plane-wave Density Functional Theory

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Charged calculations in plane-wave density functional theory (DFT) tend to be handled under the physical assumption that any net charge is compensated far from the simulation area, which is a non-local correc- tion. This understanding has resulted in varieties of boundary corrections appearing in literature[1,2,4–6] Non-local corrections are often reasonable models. However, in the case of surfaces, the electrostatic environment is, in many cases, far more complex. Any number of ions, electrolytes, or po- lar molecules may be present and would allow for some level of local com- pensation or screening. Therefore, non-local compensation schemes may require augmentation in more nuanced electrostatic environments. Here, we present how local (VASPsol)[3] and non-local compensation mechanisms (Freysoldt-Neugebaur)[2] are best considered in tandem when studying charged surfaces in plane-wave DFT.

References

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