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**Implicit solvent models in VASP** KIRAN MATHEW, Cornell university, RICHARD HENNIG, University of Florida — Solid-liquid interfaces are at the heart of many modern-day technologies and presents challenge for materials simulation methods. A realistic first-principles computational study of such systems entails the inclusion of solvent effects. In our previous work, employing a linear implicit solvent model, we have demonstrated the importance of the inclusion of solvent effects on the calucaltions of reaction energy barriers and surface enegies of semiconductor nanocrystals. In this work we propose to extend the implicit solvent model to incorporate the effects of the ions in the solvent and also to include the effects of dilectric saturation phenomenon. A solvation model that includes the effects of ionic solution at a first principle level, takes us one step closer to a more realistic simulation of an electrochemical interface. Incorporating the dielectric saturation effects futher advance the capabilities of the state of the art DFT tools to study the Solid Electrolyte Interface(SEI) films formed on highly ionic surfaces such as Lithium halides.

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