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Polarizable Force Fields for Ionic Liquid-Graphite Interfaces

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Force fields that are specifically parameterized for performing molecular dynamics simulations of liquid/solid interfaces are in high demand. Most often, the liquid/solid interactions are modeled by combining existing force fields for both phases using mixing rules. Ionic liquids (ILs) exert strong electric fields on the surrounding molecules, and therefore, are often best described using polarizable force fields.

On this poster, we present the derivation of polarizable force fields for the simple ionic liquid ([C1C1Im][BF4] at a graphite interface.[1] While building upon existing polarizable force fields for the IL[2] and graphite[3,4], we explicitly parametrize the ionic liquid/graphite interaction instead of relying on mixing rules. Implementing the derived force fields, we observe that the explicit parametrization significantly affects the structure of the interface, resulting in the formation of a sharply defined contact layer and notably reduced ion-graphite distances when compared to mixing rules-based force fields. Upon calculating the work of adhesion of the ionic liquid on graphite, we show that the liquid/solid interactions are dominated by dispersive interactions while induction effects only play a minor role. Additionally, we find that using mixing rules strongly under predicts the overall work of adhesion, highlighting the demand for and justifying the computational efforts of explicitly parameterizing the ionic liquid/graphite interactions.

References

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Tom Frömbgen is a PhD student in Theoretical Chemistry with Prof. Barbara Kirchner at University of Bonn, Germany. In his research, he uses classical, polarizable and ab initio molecular dynamics simulations to study the structure, dynamics and vibrational spectroscopy of ionic liquids. He holds a PhD scholarship of the German Academic Scholarship Foundation (Studienstiftung) and recently spent four months at MIT with Prof. Daniel Blankschtein.