Ionization and solvation in organic solvents

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Redox reactions in electrolyte solutions depend in the solvation and ionization properties of the solvent and ions. The interplay between the solvation and ionization of lithium ions in varius organic solvents is simulated using electron density functional theory (DFT) and simplified models. It is demonstrated, that, overall, DFT is able to predict redox properties of litium ions in organic solvents. However, there are a few exceptions that requre additional treatment if the litium solvatoin shell during the ionization. A universal approach of the solvation shell inclusion in the simulation is presented.
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