## Energetics of Aqueous Alkali and Halide Ions and the Hydrated Electron in Bulk Water and at the Water-Vapor Interface

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## Abstract

The vertical binding energies (VBEs) and detachment energies (VDEs) of aqueous alkali and halide ions and the aqueous electron in bulk water and at the water-vapor interface have been computed using long-range-corrected density functional theory and two continuum solvation models, one of which allows for arbitrary dielectric boundary conditions. Quantitative agreement with recent liquid microjet experiments of VBEs and VDEs for the bulk species suggests that the chosen methodologies provide reasonable models for the ions and excess electron. The VBEs and VDEs of the interfacial ions and electron are found to be very similar to those in the bulk. Our results provide insight for processes ocurring at aqueous/biological interfaces such as dissociative electron attachment.