Abstract Submitted
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Ab initio Determination of Formation Energies and Charge Transfer Levels of Charged Ions in Water. ANOOP KISHORE VATTI, MIRA TODOROVA, JOERG NEUGEBAUER, Department for Computational Materials Design,Max-Planck-Insitut fuer Eisenforschung GmbH, Duesseldorf, Germany — The ability to describe the complex atomic and electronic structure of liquid water and hydrated ions on a microscopic level is a key requirement to understand and simulate electro-chemical and biological processes. Identifying theoretical concepts which enable us to achieve an accurate description in a computationally efficient way is thereby of central importance. Aiming to unravel the importance and influence of different contributions on the hydration energy of ions we perform extensive ab-initio molecular dynamics simulations for charged and neutral cations (Zn, Mg) and anions (Cl, Br, I) in water. The structural correlations and electronic properties of the studied ions are analysed and compared to experimental observations. Following an approach inspired by the defect chemistry in semiconductors [1] and aligning the water band edges on an absolute scale allows us to benchmark the calculated formation energies, identify transition states and compare the results to experiment. Based on these results we discuss the performance of various DFT xc-functionals to predict charge transfer levels and photo-emission experiments [2]. [1] M. Todorova and J. Neugebauer, Phys. Rev. Applied 1, 014001 (2014). [2] B. Winter et al., JACS 127, 7203 (2005).

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