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Electronic Structure at Electrode/Electrolyte Interfaces in Magnesium based Batteries JANAKIRAMAN BALACHANDRAN, DONALD SIEGEL, University of Michigan, Ann Arbor — Magnesium is a promising multivalent element for use in next generation electrochemical energy storage systems. However, a wide range of challenges such as low coulombic efficiency, low/varying capacity and cyclability need to be resolved in order to realize Mg based batteries. Many of these issues can be related to interfacial phenomena between the Mg anode and common electrolytes. Ab-initio based computational models of these interfaces can provide insights on the interfacial interactions that can be difficult to probe experimentally. In this work we present ab-initio computations of common electrolyte solvents (THF, DME) in contact with two model electrode surfaces namely — (i) an "SEI-free" electrode based on Mg metal and, (ii) a "passivated" electrode consisting of MgO. We perform GW calculations to predict the reorganization of the molecular orbitals (HOMO/LUMO) upon contact with the these surfaces and their alignment with respect to the Fermi energy of the electrodes. These computations are in turn compared with more efficient GGA (PBE) & Hybrid (HSE) functional calculations. The results obtained from these computations enable us to qualitatively describe the stability of these solvent molecules at electrode-electrolyte interfaces

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