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Corrosion Thermodynamics of Magnesium and Alloys from First Principles as a Function of Solvation KRISTA LIMMER, US Army Rsch Lab - Aberdeen, KRISTEN WILLIAMS, Boeing, JAN ANDZELM, US Army Rsch Lab - Aberdeen — Thermodynamics of corrosion processes occurring on magnesium surfaces, such as hydrogen evolution and water dissociation, have been examined with density functional theory (DFT) to evaluate the effect of impurities and dilute alloying additions. The modeling of corrosion thermodynamics requires examination of species in a variety of chemical and electronic states in order to accurately represent the complex electrochemical corrosion process. In this study, DFT calculations for magnesium corrosion thermodynamics were performed with two DFT codes (VASP and DMol3), with multiple exchange-correlation functionals for chemical accuracy, as well as with various levels of implicit and explicit solvation for surfaces and solvated ions. The accuracy of the first principles calculations has been validated against Pourbaix diagrams constructed from solid, gas and solvated charged ion calculations. For aqueous corrosion, it is shown that a well parameterized implicit solvent is capable of accurately representing all but the first coordinating layer of explicit water for charged ions.

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