A FIRST PRINCIPLES INVESTIGATION OF THE OXYGEN ADSORPTION TO THE ZR(0001) SURFACE USING THE CLUSTER EXPANSION METHODOLOGY

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ABSTRACT

The design of corrosion resistant zircalloys is important for a variety of technological applications ranging from medicine to the nuclear industry. Since corrosion resistance is mainly attributed to the formation of a surface oxide layer, developing a detailed understanding of this process is of crucial importance. In this work, we conduct a systematic and multi-scale investigation of the early stages of oxide formation. This is accomplished by first using a DFT-database to build a cluster-expansion description of the potential function describing the interactions in the adlayer. The developed potential was reasonably good at predicting DFT energies as evidenced by the cross-validation score. The potential then allowed for a systematic investigation of the oxygen configurations on the Zr(0001) surface via Monte Carlo simulations. The convex hull diagram was recorded indicating the most stable configuration at each coverage and the adsorption isotherm was also recorded.