

First Principles Investigation of Corrosion Mechanisms in Austenitic Steel Alloys

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Austenitic steel alloys are the material of choice for a wide range of industrial applications. Their robust mechanical properties, cost effectiveness, and superior corrosion resistance put this class of materials in high demand for manufacturers who strive to push the limit of performance with their components. As the demands of the technical applications for these alloys become increasingly stringent, a deeper understanding of their potential failure mechanisms is required to optimize performance. This optimization process begins at the materials-scale where atomistic properties and the thermodynamics of reaction mechanisms can be evaluated to offer insight that provides a fundamental physical grounding for the development of these enhanced components. In this work, density functional theory is employed to calculate the energy cost of defect formation and migration in the experimentally observed oxide compounds which form atop austenitic steel alloys when exposed to elevated temperatures (>700 °C). From these calculations, a model of the most likely corrosion mechanisms which accounts for both thermodynamic and kinetic viability is established. Of particular interest, is the MnCr_2O_4 spinel phase which has been shown experimentally to form as an intermediate layer in the composite oxide film. This compound's mediating position between bulk alloy and outermost oxide layer offers a wealth of chemical complexity to explore. As such, a comprehensive analysis of the defect migration pathways in this system is central to the development of an overarching corrosion model.