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Developing an Ab Initio-Kinetic Model for the Prediction of Passivation Behavior[1] RACHEL GORELIK, PETER CROZIER, ARUNIMA SINGH, Arizona State University — With the US economy incurring $200 billion annual losses due to corrosion, there is still a significant need for effective a priori models which enable the prediction of materials' corrosion resistance, particularly within the field of materials discovery. While most current predictive models use fully empirical parameters, there is a value in the development of kinetic models which utilize solely quantum-mechanics-derived inputs. As a first step in this direction, we therefore develop an ab initio-kinetic model by applying the Pilling-Bedworth Rule (PBR), a metric commonly used to predict the passivation protectiveness of a given material based on mechanical driving forces. With a previously developed ab initio methodology for determining the passivation products of any material, we automate a methodology utilizing the PBR for all materials currently in the Materials Project database, and furthermore we extend it to include materials which are predicted to form more than one passivation product on their surfaces. Upon development, this model can serve as a preliminary, low-cost screening step which can be applied to any material for predicting its electrochemical stability.

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