

## Corrosion-resistant Mg alloy design through high-throughput simulations and machine learning

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**Abstract** Magnesium alloys as the lightest engineering metals have the potential to be widely used in transportation etc, but the bad corrosion resistance has limited the further applications. To overcome the limitations of traditional experimental trial-and-error approach in corrosion research, the ab-initio method to predict the polarization curves for galvanic corrosion of multi-phase Mg alloys has been established. To accelerate the screening of Mg alloy systems with better corrosion resistance, the corrosion materials genome have been further developed by combining the high-throughput-simulations and machine learning methods. The important surface atomic features have been also uncovered in terms of reducing the cathodic hydrogen evolution and anodic Mg dissolution kinetics, which have successfully guided the experimental development of corrosion-resistant Mg alloys.

**Keywords** High-throughput simulations; Materials Genome Initiative; Corrosion property; Machine Learning

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