

## Artificial intelligence combined with high-throughput calculations to improve the corrosion resistance of AlMgZn alloy

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**Abstract** Efficiently designing lightweight alloys with combined high corrosion resistance and strength remains an enduring topic in materials engineering. To this end, machine learning (ML) coupled ab-initio calculations is proposed within this study. Due to the inadequate accuracy of conventional stress-strain ML models caused by corrosion environment factors, a novel reinforcement self-learning ML algorithm (accuracy  $R^2 > 0.92$ ) is developed. Then, a strategy that integrates ML models, calculated energetics, and mechanical properties is implemented to optimize the Al alloys. Next, this Computation Designed Corrosion-Resistant Al alloy is fabricated that verified the simulation. The performance (elongation reaches ~30%) is attributed to the H-captured Al-Sc-Cu phases and Cu-modified  $\eta/\eta'$  precipitation inside the grain boundaries (GBs). The trained Al-Mg-Zn-Cu interatomic potential (energy accuracy 6.50 meV/atom) proves the cracking resistance of GB region enhanced by Cu-modification. Conceptually, our strategy is of practical importance for designing new alloys exhibiting combined exceptional properties.

**Keywords** Al-Zn-Mg alloys; Machine learning; first-principles calculation; molecular dynamic simulation; Precipitates;

### Reference

[1] Yucheng Ji, X. Fu, et al., Artificial intelligence combined with high-throughput calculations to improve the corrosion resistance of AlMgZn alloy, Corrosion Science. 233 (2024) 112062.

[2] Yucheng Ji, C. Dong, et al., High-throughput computing for screening the potential alloying elements of a 7xxx aluminum alloy for increasing the alloy resistance to stress corrosion cracking, Corrosion Science, 183 (2021) 109304.