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Magnesium-Silicon Alloy Phase Stability Predictions: A cluster expansion study.

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Rechargeable batteries have the potential to help meet the ongoing demand for portable energy and to mitigate the energy crisis in countries such as South Africa. These call for the accelerated development of novel and advanced high-energy battery electrode materials. Magnesium-Silicon (Mg-Si) anodes have emerged as attractive alternatives to the graphitic anodes used in current lithium-ion battery technologies. However, the commercialisation of batteries based on the Mg-Si alloy is deterred by a few obstacles including the incompatibility of the Mg-Si anode with conventional battery electrolytes. In this work, the material space of the Mg-Si alloy system was explored through crystal structure predictions conducted via a machine learning (ML) powered cluster expansion technique (CE). The aim was to predict and analyse novel and stable phases of the magnesium-silicon alloy system whose compatibility with electrolytes shall be interrogated in future work. The genetic algorithm embedded within the CE technique was used to accelerate the material discovery process by performing the ground-state search of stable structures from the Mg-Si alloy system. By considering the BCC and FCC-based parent lattice, 8 structures were predicted to be thermodynamically stable, namely, Mg₅Si (Imma), Mg₂Si (P-3m1), MgSi (P4-mmm), Mg₃Si (Pm-3m), MgSi₃ (Pm-3m), MgSi₃ (P2-m), MgSi (Im-3m), and Mg₃Si (P4/mmm). The geometric properties of these structures are presented. From the predicted structures, the orthorhombic magnesium-rich phase, Mg₅Si, was found to be structurally stable and a promising candidate for Mg-Si-based rechargeable batteries. The findings from this study are crucial to the advancement of high-energy battery electrode materials for next-generation batteries.

Apply to be considered for a student ; award (Yes / No)?

No

Level for award;(Hons, MSc, PhD, N/A)?

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