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Cluster expansion calculations on the discharge product of magnesium-ion batteries

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Magnesium batteries have poor cycle performance, which limits their commercial use. In magnesium batteries, sulphur (S) performs poorly and reduces the battery's performance; however, when selenium (Se) is added, the issue is improved and the material's energy density is enhanced. Therefore, in this study, cluster expansion technique was employed to determine phase changes of mixed MgSc2S1-xSex, MgY2S1-xSex, and MgIn2S1-xSe systems, which then generated 97, 61, and 12 new mixed phases, respectively. Furthermore, the potential of Se, a d-electron possessing periodic table element with excellent electrical conductivity, as an electrode material for rechargeable magnesium batteries is explored. The systems created a miscibility gap, leading to the introduction of Monte Carlo simulations. Monte Carlo simulations produced thermodynamic properties for Se concentrations obtained from cluster expansion, and it demonstrated that all the systems are phase separating at 0K. Temperature was varied and the systems changed to mixed systems at an approximately 250K-400K range. Finally, Monte Carlo simulations yielded consistent results on phase separation and high-temperature behaviour for all the systems at 50% sulphur and selenium.

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

Yes

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

PhD

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