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# Ab initio and Cluster Expansion study on Magnesium Spinel (MgX2Z4: where X=Sc, Y and In; Z=S and Se)

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Magnesium-ion batteries are facing major setbacks when it comes to the identification of cathode materials which will demonstrate capacities and voltages identical to lithium-ion systems. Then, in this study, we make use of first-principle based calculations to study the stability of the discharge products MgSc2S4, MgSc2Se4, MgY2S4, MgY2Se4, MgIn2S4, and MgIn2Se4 whereby we investigate their structural, mechanical, and electronic properties, and their phase stability. Computational technique was employed utilising the ab initio density functional theory through the Vienna Ab initio Simulation Package code within the generalised gradient approximation in the form of Perdew-Burke-Ernzerhof exchange correlation. Heats of formation shows that all structures are stable. Calculated elastic constants indicate that the structures are mechanical stable which is in good agreement with the phonon dispersion curves. The total density of states indicates that all structures are semi-conductors. Phonon dispersion curves shows that the structures are vibrational stable due to no soft modes observed along the gamma region. Following these discoveries, we employed the Universal Cluster Expansion code, which is a machine learning code. We added Selenium to Sulphur since Selenium has the advantage of prolonging the lifespan of S. It is found that MgSc2S1-xSex, MgY2S1-xSex, and MgIn2S1-xSex systems, generated 97, 61, and 12 new mixed stable phases, respectively. Now the results found in this study aimed to give an insight on the stability of solid electrolytes and in order to provide inspiration for future Research and Development in magnesium-ion batteries.

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

Yes

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

MSc

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