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Computational modelling on Stability of Solid Electrolytes in Magnesium ion batteries

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Developing new battery technologies to sustain the ever growing demand of energy storage constitutes one of the greatest scientific and societal challenges of the century. Lithium-ion batteries (LIBs) are at the center of energy revolution, they power millions of portable electronics and electric vehicles. Li ion's success is in part due to the remarkable mobility of Li⁺ in many solids. Fast Li-ion transport enables intercalation electrodes, in which charge is stored by moving the ions in and out of crystal structures. A technology that has the potential to alleviate resource issues with Li-ion systems and further increase the energy density is Mg²⁺ intercalation systems. Replacing Li with safer and earth abundant Mg has the advantage of doubling the total charge per ion, resulting in larger theoretical volumetric capacity compared with typical LIB. Most importantly, in Mg batteries, the anode is constituted by energy dense Mg metal notably surpassing the theoretical volumetric energy density of the current graphitic anode of LIB and even that of lithium metal. In this study we investigate by using first principle calculations within generalized gradient approximation the stability of MgSc₂S₄ and MgSc₂Se₄ structures. The lattice parameters are in good agreement with experimental studies. The heats of formation indicate that the structures are stable. Calculated elastic properties shows that structures are mechanically stable.

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