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Examining the structural, mechanical and electronic properties of Si-C composite for next-generation anode material

Anode materials used in lithium-ion batteries have gained enormous interest in research due to their high Coulombic efficiency and cost-effectiveness. Commercially, graphite is used as the anode material due to its stability but exhibits a low capacity of 372 mAh/g (LiC6). Silicon has attracted attention because of its high theoretical capacity of 4200 mAh/g (in Li4.4Si), making it a promising candidate for next-generation batteries. However, its volume expansion during the lithiation and de-lithiation processes is a major drawback since it causes loss of electrical contact and low coulombic efficiency. To enhance silicon structural stability and remedy the issues of electrochemical performance, designing silicon composites could work. In this study, the cluster expansion technique is used to determine new and stable variants of Si-C alloy of space group Fd-3m. The cluster expansion simulation produced 25 new structures, with a cross-validation score (CVS) of 6.1 meV/pos. The SiC structure appears on the DFT ground state line which indicates that the structure is thermodynamically stable and has the lowest heat of formation. The structure was found to be cubic in symmetry and mechanically stable. The density of states and band structure of SiC shows an indirect band gap of 1.37 eV which suggests semi-conductor behavior. The findings of this research will contribute to determining a new stable Si-based composite, which will advance the anode materials for next-generation rechargeable batteries.

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