Contribution ID: **325** Type: **Poster Presentation**

Fe-Doped $NaVS_2$: A Study on the Structural, Electronic, and Electrochemical Properties for Enhanced Energy Storage Applications

Abstract

The transition metal dichalcogenide (TMD) $NaVS_2$ has attracted considerable attention as a candidate for energy storage systems, particularly sodium-ion batteries (SIBs), owing to its excellent electrical conductivity, advantageous electronic properties, and catalytic versatility. Nevertheless, its practical application is hindered by limited ionic conductivity and suboptimal cycling stability. In this work, we explore how iron (Fe) doping influences the structural, electronic, and electrochemical characteristics of $NaVS_2$ to enhance its performance as an energy storage material. First-principles calculations based on density functional theory (DFT) were used to analyse the electronic band structure, density of states (DOS), and formation energies. The findings reveal that incorporating Fe significantly alters the electronic behavior, resulting in a reduced band gap and increased DOS at the Fermi level, both beneficial for facilitating rapid charge transport. The negative formation energies further indicate the thermodynamic feasibility of Fe substitution in the $NaVS_2$ lattice. These structural and electronic enhancements are likely to improve ion mobility and electrode longevity under repeated cycling. Furthermore, the study sheds light on how dopant type and concentration can be strategically utilized to optimize TMD materials for energy-related applications. In conclusion, Fe-doped $NaVS_2$ shows strong promise as an advanced electrode material for SIBs, and the findings reinforce the broader potential of transition metal doping in fine-tuning TMD properties for battery technologies.

Keywords: sodium-ion batteries, transition metal dichalcogenides, density functional theory, electronic structure.

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Session Classification: Poster Session

Track Classification: Track A - Physics of Condensed Matter and Materials