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Density functional theory study of Nax (TiyZnzMnw)O2 as a cathode material

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Rechargeable sodium-ion batteries have attracted great attention for large-scale electric energy storage applications and smart grid owing to the abundance of Na resources and comparable performance with lithium-ion batteries. The use of organic electrode materials enables a sodium storage system with high energy/power density, metal-free, environmental friendliness, flexibility, lightweight, and cost-effectiveness has recently attracted tremendous research interest. In this study, density functional theory was used to investigate structural and electronic properties NaMnO2 doped with Ti and Zn. expansion of volumes is induced by the dopants, The partial density of states underlines that these states nearby the Fermi level are contributed from the d-orbital of Ti and Zn. The magnetism is attributed from the hybridisation of d-orbitals of dopant and Mn atom with O-p states, namely p-d exchange hybridisation. The lowest conduction band and highest valence band are mostly contributed from Mn atom, Ti and Zn dopants which are responsible for the electronic conductivity. Na(Mn,Ti)O2 and Na(Mn,Zn)O2 and are all semiconductors with reduced band gaps, while Na(Mn,Ti,Zn)O2 displays half-metallic ferromagnetic behavior.

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

YES

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

PhD

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