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Density functional theory study of Ni doped NaMnO2 cathode material

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Rechargeable sodium-ion batteries (SIBs) 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, in this study Density functional theory (DFT) has been used to study the electronic (band structure & TDOS), Elastic properties and intercalation voltage of NaMnO2 doped with Ni.The generalized gradient approximation (GGA) was used in the scheme of Perdew-Burke Ernzerhof to describe the exchange -correlation function as implemented in the CASTEP package in material studio of BIOVIA. Our findings show that NaMnO2 possess high voltage window and a good reversible capacity. The elastic properties shows that NaMnO2 doped with Ni is stable, while the electronic properties shows that metallicity of NaMnO2 gradually increases during Na extraction

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

Yes

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

PhD

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