



Contribution ID: 287

Type: **Oral Presentation**

## Density functional theory study of Ni doped NaMnO<sub>2</sub> cathode material

*Thursday, 29 July 2021 15:00 (15 minutes)*

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 NaMnO<sub>2</sub> 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 NaMnO<sub>2</sub> possess high voltage window and a good reversible capacity. The elastic properties shows that NaMnO<sub>2</sub> doped with Ni is stable, while the electronic properties shows that metallicity of NaMnO<sub>2</sub> 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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**Session Classification:** Applied Physics

**Track Classification:** Track F - Applied Physics