Canadian Association of Physicists
Association canadienne des physiciens et physiciennes

Contribution ID: **2051** Type: **Oral (Graduate Student) / Orale (Étudiant(e) du 2e ou 3e cycle)**

Impact of aluminum substitution on the electronic and thermodynamic properties of NCA materials for lithium-ion batteries using first-principles methods (G)

Tuesday 12 June 2018 16:00 (15 minutes)

Tuning positive electrode materials in lithium-ion cells provides a promising means for lowering cost of materials while maintaining safety and energy density standards. Due to the rising cost of cobalt, it is important to find less expensive alternatives. Here we present results from first-principles computations within the formalism of density functional theory examining changes in electronic properties and thermodynamic stability of $Li_xNi_{1-y-z}Al_yCo_z$, where $0x1$ and $0y$, $z0.2$, positive electrode materials as a function of cobalt, aluminum, and lithium content. Results using a new exchange-correlation functional (SCAN) [1,2] within the class of meta-GGAs are compared with the traditionally employed empirical GGA+U. Fundamental understanding of these properties may help in designing less expensive positive electrode materials.

[1] Strongly Constrained and Appropriately Normed Semilocal Density Functional, J. Sun, A. Ruzsinszky, and J.P. Perdew, Phys. Rev. Lett. 115, 036402 (2015)
[2] Accurate first-principles structures and energies of diversely bonded systems from an efficient density functional, J. Sun et al., Nature Chemistry 8, 831–836 (2016)

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Session Classification: T4-1 Energy Storage 2 (DCMMP) | Accumulation 2 (DPMCM)

Track Classification: Condensed Matter and Materials Physics / Physique de la matière condensée et matériaux (DCMMP-DPMCM)