Contribution ID: **162** Type: **Poster**

【631】Charge localization and energetics of Li-ion batteries cathodes from extended Hubbard-corrected functionals

Wednesday 23 August 2017 12:30 (1 minute)

The accurate modeling of transition-metal compounds (TMC) is essential for their deployment as electrodes of Li-ion batteries.
Allowing to capture the localization of electrons during charge/discharge, Hubbard-augmented DFT functionals (DFT+U) have become the standard choice for the modeling of TMC when computational efficiency is required. This work shows how an extended formulation of DFT+U, including on-site (U) and inter-site (V) interactions, improves the description of the equilibrium structure and the electronic properties of mixed valence cathode materials as Li_xMPO_4 and Li_xCoO_2. In particular, the use of computed interaction parameters is shown to be crucial to assess the stability of intermediate compositions and to evaluate the voltage of the battery.

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Session Classification: Poster Session

Track Classification: Correlated-Electron Physics in Transition-Metal Oxides