Contribution ID: **249** Type: **Poster Presentation**

Optimising Buckingham interatomic potentials for use in molecular dynamics using DFT total energies Na-doped Li-rich Li1.2Mn0.8O2 Cathode Simulation

In the current study, we are exploring the Li-rich cathode material Li2MnO3 which is generally electrochemically passive. Li2MnO3, as a Li-ion and structural stabilizer, can offer higher capacity and is thought to be a promising alternative to traditional cathode materials, such as LiCoO2, in the form of Li-rich Mn-based layer-structured oxides, xLi2MnO3-(1-x)LiMO2 (M = Ni, Co, Mn, etc.). we have constructed the Li1.2 Mn 0.8 O 2 structure from Li2MnO3 with space group R-3m, and intend to study the effect of doping Li with Na on the properties of the nanostructured Li-rich Li1.2Mn0.8O2 cathode. The interatomic potentials of Li were available, except for those of the Na-Li interaction. We calculated the properties of LiNaO using DFT for fitting the Na-Li potential parameter as there were no experimental properties in the literature. We calculated the short-ranged repulsive potential of Na-Li from the DFT total energies of the LiNa system, fitted the Buckingham potential parameters to it, and obtained A = 28250.5, ρ = 0.231, and C = 0. These interatomic potential parameters were used as a starting point in GULP and further fitted against the DFT-calculated properties of the LiNaO structure and obtained A = 38500.5, ρ= 0.177,and C = 0. The obtained Li-Na Buckingham interatomic potential parameters in conjunction with existing interatomic potentials for O-O, Li-O, Li-Li, Na-O, Na-Na reproduced the lattice parameters a=b and c of LiNaO to within 1.52 and -1.7 %, respectively. The elastic constants obtained were reasonable when compared to their DFT values. Fitting the initial Buckingham interatomic parameters to the repulsive potential greatly reduced the fitting time. The deduced potentials are then going to be used to amorphize and recrystallize the doped Na-Li 1.2 Mn 0.8 O 2 structure.

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Session Classification: Poster Session

Track Classification: Track A - Physics of Condensed Matter and Materials