Contribution ID: **210** Type: **Oral Presentation**

Derivation of empirical interatomic potentials for interactions that emanate from doping Li-Mn-O spinel with nickel and cobalt.

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Molecular dynamics (MD) simulations which generally rely on empirically parameterized functions are currently the only practical option for large-scale computational studies of materials. The process of determining these parameters is quite a challenge, particularly given that the final potential parameters are extensively dependent on the initial parameters. Hence, finding initial parameters that are linked to the physical characteristics of the interaction is pivotal to the process, as such, we employ a machine-learning technique (to determine initial parameters) and the General Utility Lattice Program (GULP) (to determine final parameters) to develop accurate Buckingham interatomic potentials for interactions that arise from doping Li-Mn-O spinel with Co or Ni. The potentials will enable the correlation of various properties linked to the electrochemical performance of the Li-M-O spinel (M = Mn, Co, Ni) cathode materials to their microstructural changes through large-scale MD simulations. The exploration will provide insights on how to curtail the reported capacity fading of Li-Mn-O spinel which is a promising cathode material for lithium-ion batteries. A curve_fit function of the SciPy library was used to determine the initial potential parameters, which are thereafter refined with GULP. Moreover, the developed potentials are tested by performing MD simulations with the DL_POLY code. The final Buckingham potential parameters for all the interactions that arise from doping Li-Mn-O spinel with Ni and Co were successfully derived. The fitted and calculated lattice parameters were comparable with a percentage difference of less than 4 %. X-ray Diffraction (XRD) graphs of the simulated spinel structures (LiCo2O4, LiNi2O4, LiMn1.875Ni0.125O4, and LiMn1.875Co0.125O4) showed the presence of the LiM2O4 and M3O4 (M = Mn, Co, Ni) phases which are in line with findings in literature. The RDF graphs of the doped structures show that doping Li-Mn-O spinel with Co could enhance structural stability.

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

Yes

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

PhD

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