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Machine Learned Buckingham Interatomic Potentials for Co-doped Li-Mn-O spinel.

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The current operational materials for lithium-ion batteries require improvement to sufficiently support large-scale systems such as the revolutionary electric vehicles and the storage of the sporadic energy garnered from renewable energy sources. Spinel LiMn2O4 is one of the safest and economically viable cathode materials that can provide adequate energy densities. However, LiMn2O4 suffers capacity fading during prolonged charge/discharge cycles. First-principles studies have shown that cation doping is one of the most effective ways of improving material performance. The effect of doping spinel LiMn2O4 at both electronic and atomic-level is not yet fully understood, particularly with Co, Ni, Cr, and Zr. The atomic-level exploration of such doping of LiMn2O4 to yield insights on how to suppress the reported capacity fading is hindered by the lack of accurate interatomic potentials. Hence, in this study we employ machine learning technique and the General Utility Lattice Program (GULP) to develop accurate Co – Co, Co - O and Co – Mn Buckingham interatomic potentials to be incorporated in a Co-doped Li-Mn-O spinel. The Buckingham potentials for Co – Co and Co – O interactions have been developed successfully and used to perform the molecular dynamics (MD) technique Amorphisation and Recrystallisation (A&R). The Co – Co and Co – O potentials have been tested on LiCo2O4 which successfully amorphised at 1900 K and recrystallised at 1900 K. The generated potentials will enable the exploration of the effect of doping nanostructured Li-Mn-O spinel with cobalt on the operating voltage which directly affects the energy density of battery.

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yes

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PhD

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