Contribution ID: **148** Type: **Poster Presentation**

First-Principles Study of Nb/Mn Doping on $LiNiO_2$ (101) Surface And It's Interaction With Ethylene Carbonate

Nickel-rich layered materials such as $LiNiO_2$ offer high energy density, making them strong candidates for next-generation lithium-ion battery cathodes. However, their structural instability remains a critical challenge. In this study, spin-polarized density functional theory calculations [DFT + U-D3 (BJ)] were employed to investigate the effects of Nb and Mn doping on the first and second layers of the $LiNiO_2$ (101) surface. Surface free energy calculations reveal that doping lowers surface energy compared to the pristine surface, indicating enhanced surface stability. Furthermore, Nb doping in the second layer provides greater stabilization than in the first layer, while Mn doping is more effective in the first layer. Bader charge and work function analyses suggest that surfaces with second-layer doping exhibit higher reactivity at the topmost layer. Ethylene carbonate (EC) adsorption on both pristine and doped surfaces yielded negative adsorption energies, confirming thermodynamic stability. Among the investigated sites, adsorption at the Ni_{23} site showed the strongest interaction, with the most negative adsorption energy. These findings provide insight into the role of Nb and Mn dopants in tuning surface stability and reactivity of $LiNiO_2$ cathodes, with implications for improved electrolyte interaction and battery performance

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Session Classification: Poster Session

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