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First-Principles Study of Mn-Doped $LiNiO_2$ (101) Surface and Its Interaction with Ethylene Carbonate Electrolyte

Nickel-rich layered metal oxides, such as $LiNiO_2$, are among the most promising cathode materials for next-generation lithium-ion batteries due to their high energy density. Doping is widely recognized as an effective strategy to enhance their structural stability and electrochemical performance. However, a detailed understanding of the role played by individual dopants is essential for rational material design. In this study, spin-polarized density functional theory calculations [DFT + U-D3 (BJ)] were conducted to examine the effect of Mn doping on the first and second layers of the $LiNiO_2$ (101) surface. The surface free energy is lower when Mn is incorporated into the first layer, implying that first-layer doping offers more effective surface stabilization than second-layer doping. Bader charge analysis shows a lower charge on Mn in the first layer, while a higher work function is observed, indicating that the surface doped in the second layer is more reactive at the outermost layer. Additionally, ethylene carbonate (EC) adsorption at various Ni sites on both pristine and doped surfaces yielded negative adsorption energies, confirming thermodynamic favorability. Among these, the Ni_{23} site exhibited the most negative adsorption energy, suggesting a stronger interaction between EC and the surface.

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