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# First-Principles Study on the Role of Ti, V, and Sc Catalysts in Enhancing the Catalytic Effects of Boron Oxide Monolayer for Efficient Lithium-Selenium Batteries

Ongoing research on lithium-air batteries aims to overcome setbacks caused by shuttle effects by exploring various cathode materials, with a particular focus on 2D materials such as monolayer boron oxides (MBOs).These materials are gaining popularity due to their unique properties, such as large surface areas, ballistic electronic transport, mechanical strength, and anisotropy, making them promising candidates for cathodes in lithium-air batteries. In this study, density functional theory (DFT) implemented within the quantum espresso code was employed to investigate the interaction of lithium polyselenides (specifically $Li_2Se_x$, where x = 1, 2, 4, 6, and 8, as well as $Se_8$) with monolayer boron oxide (MBO). We investigated the influence of lithium polyselenides on monolayer boron oxide (MBO), focusing on adsorption energy, charge density distribution, Gibbs free energy changes, and metallic characteristics for efficient lithium-selenium batteries. The initial results showed that the adsorption energies of these lithium polyselenides on pristine MBO are relatively weak, ranging from -0.25 to -1.43 eV. In contrast, doping MBO with scandium (Sc) significantly increased the adsorption energies, ranging from -2.65 to -3.74 eV, indicating a notable enhancement compared to other tested single-atom catalysts (SACs). The higher adsorption energy of Sc-doped MBO suggests an improved ability to prevent the dissociation of lithium polyselenides into the electrolyte, which is critical for addressing the shuttle effects. Charge density distribution analyses further support the presence of electronic interactions between the substrate and the adsorbed lithium polyselenides via Sc catalysts, as evidenced by charge transfer from the adsorbate to the substrate. Additionally, the investigation of Gibbs free energies revealed low charge, discharge, and overpotential values (0.1 V for pristine MBO and 1.53 V for Sc-doped MBO). The Sc-doped MBO structure exhibits significantly enhanced metallic characteristics after the adsorption of $Li_2Se$ and $Li_2Se_4$. Furthermore, the low diffusion (1.56 eV) and dissociation (1.72 eV) energy barriers for stable $Li_2Se$ on Sc-doped MBO suggest the material's potential to improve electrochemical processes and enable higher charging rates in lithium-selenium batteries. Ultimately, while pure MBO alone may not effectively address the challenges associated with lithium-selenium batteries, doping it with Sc substantially enhances its properties as a cathode material.

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**Primary author:** MAPASHA, Edwin (University of Pretoria)

**Co-authors:** Mr FWALO, Chewe (University of Pretoria); Dr IGUMBOR, Emmanuel (University of Johannesburg)

**Presenter:** MAPASHA, Edwin (University of Pretoria)

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