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Electronic structure and electrochemical properties of Li/Na-adsorbed $ZnCo_2O_4$ for Li- and sodium-ion batteries

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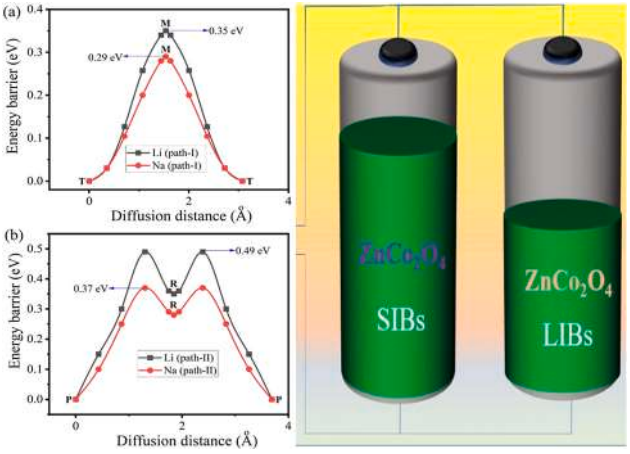
HIGHLIGHTS

- Li/Na adsorption boosts $ZnCo_2O_4$ conductivity, enabling high-energy anodes for next-gen sodium-ion batteries.
- Mesoporous $ZnCo_2O_4$ enables fast electron transport and volume stability.
- Low Li/Na diffusion barriers (0.35/0.29 eV) support efficient ion transfer.

GRAPHICAL ABSTRACT



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ABSTRACT

First-principle calculations are used to analyze the electronic structure and electrochemical properties of Li/Na-adsorbed $ZnCo_2O_4$ for Li- and Na-ion batteries. Li/Na adsorption increases its electrical conductivity at lower

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