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ABSTRACT:

Mg and Zn migration in cation defective spinel-type MgxZnMnO3

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We investigated Mg insertion in cation-defective spinel MgxZnMnO3 ($0 \leq x \leq 1$) and Mg/Zn ion transport using a neural network potential combined with molecular dynamics simulations[1,2]. Cation configurations were optimized using a genetic algorithm. The results indicate that a vacancy-driven spinel (VDS) region ($x < 0.25$) is stabilized as a solid solution, whereas a spinel–rock-salt biphasic (BSR) coexistence region is favored for $0.25 < x < 0.84$. The diffusion coefficients exhibited a strong composition dependence: both stoichiometric spinel ($x = 0.25$) and rock-salt ($x = 1.0$) phases showed extremely low ionic conductivity (< 10-10 cm2 s-1), while enhanced diffusivity was observed in the VDS and BSR regions, reaching 3.97 × 10-7 cm2 s-1 at $x = 0.50$. Zn2+ consistently diffused faster than Mg2+, and both ions migrated along identical 8a–16c–8a diffusion channels. Trajectory analysis further suggests possible concerted hopping mechanisms. These results reveal that Zn plays a dual role by stabilizing tetrahedral sites and enhancing Mg mobility. The precipitation of stoichiometric phases ($x = 0.25$ and 1.0) may hinder Mg transport and reduce capacity; however, the low energy-above-hull values suggest that solid-solution pathways are kinetically accessible. Overall, these findings provide design guidelines for achieving both high voltage and improved Mg diffusivity in magnesium battery cathodes.

References

[1] Shimokawa et al., Adv. Mater., 33, 2007439 (2021).
[2] . Nakahara et al., Chem. Asia. J. 21, e00908, (2025).