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Thermodynamic Stability of MgSc2Se4 Surfaces

Magnesium-based batteries represent a promising post-lithium battery technology due to magnesium's low cost and high natural abundance. Among the few materials exhibiting good Mg ion conductivity, the spinel phase $MgSc_2Se_4$ stands out as a particularly promising solid electrolyte candidate.[1] While the bulk properties of $MgSc_2Se_4$ are already well understood, advancing toward practical applications requires comprehensive understanding of interface behaviour in complete battery systems. This work focuses on elucidating surface stability and restructuring phenomena of $MgSc_2Se_4$. We employed periodic density-functional theory to investigate experimentally relevant surface facets, providing insights into atomic-scale behaviour at its surface. Based on ab-initio thermodynamics, we constructed a phase diagram mapping $MgSc_2Se_4$ surface stability as a function of the chemical potentials of its atomic species.[2],[3] Our results reveal the relative stability of different surface terminations and planes. These findings provide fundamental insights into $MgSc_2Se_4$ surface properties essential for understanding and optimising solid-state magnesium battery performance.

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