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2D transition metal carbides as flexible anode materials

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MXenes exhibit many outstanding properties and therefore been considered as promising electrode material candidates. Taking 2D transition metal carbides as representatives, we systematically explored several influencing factors, including transition metal species, layer thickness, functional group, and strain on their mechanical properties (e.g., stiffness) and their electrochemical properties (e.g., ionic mobility). Considering potential charge-transfer polarization, we employed a charged electrode model to simulate ionic mobility and found that ionic mobility has a unique dependence on the surface atomic configuration influenced by bond length, valence electron number, functional group, and a strain. Under multiaxial loadings, electrical conductivity, high ionic mobility, low equilibrium voltage with good stability, excellent flexibility, and high theoretical capacity indicate that the bare 2D TMCs have potential to be ideal flexible anode materials, whereas the surface unctionalization degrades the transport mobility and increases the voltage due to bonding between the nonmetals and Li.

Summary

Topic

1. Low-dimensional systems

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