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First-Principles Investigation of Cu3XN Antiperovskite Electrocatalysts for CO2 Reduction

Antiperovskite-type Cu3XN (X = Ni, Pd, Pt) materials have recently emerged as promising candidates for catalytic CO2 electroreduction due to their metallic conductivity, tunable surface chemistry, and structural flexibility. In this work, we employ first-principles density functional theory (DFT) calculations to investigate the electronic and catalytic properties of Cu3XN systems with a focus on identifying active surface terminations and understanding their role in CO2 activation. Surface energies were calculated to determine the thermodynamically preferred facets, followed by detailed electronic structure analysis through band structure, density of states (DOS), and projected DOS (PDOS) evaluations. The results reveal strong hybridization between Cu-d and X-d orbitals near the Fermi level, facilitating enhanced electron transfer essential for catalytic activity. We further evaluated key reaction intermediates and adsorption energetics along the CO2 reduction pathway, including *COOH and*OCHO species, to assess reaction feasibility and selectivity. Overall, our findings highlight the potential of Cu3XN antiperovskites as efficient electrocatalysts for CO2 conversion and provide valuable insights for the rational design of next-generation catalytic surfaces.

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