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Density functional theory-based exploration of structural, electronic, mechanical, thermodynamic, and optical properties of α-NiS for CO2 adsorption

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In this study, we performed comprehensive first-principles calculations based on density functional theory to investigate the structural, electronic, mechanical, thermodynamic, and optical properties of α-nickel sulfide (α-NiS), with a particular emphasis on its potential for CO2 adsorption. Structural optimization confirms the stability of the α-NiS phase, yielding lattice parameters, a = b = 3.425 Å, c = 5.286 Å, in good agreement with experimental data. Electronic band structure analysis reveals a semiconducting nature with a bandgap of 1.98 eV. Mechanical and thermodynamic analyses confirm the elastic and thermal stability of α-NiS, supporting its suitability for surface reactions. Optical property calculations indicate that α-NiS exhibits strong absorption across a broad spectral range, highlighting its potential in photonic and catalytic systems. To evaluate its gas adsorption capabilities, CO2 adsorption on both Ni- and S-terminated surfaces was investigated. The results show that CO2 binds more strongly to the Ni-terminated surface through ionic interactions, forming Ni–O bonds with a bond length of 2.36 Å and a bond angle of 95.5°, while interaction with the S-terminated surface is weaker and predominantly covalent. The calculated adsorption energies of -2.71 eV (Ni-side) and -0.98 eV (S-side) further confirm the thermodynamic favorability of CO2 adsorption on the Ni-terminated surface, suggesting α-NiS as a promising candidate for gas capture applications.

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