Rational Design of Nickel Nano-catalysts on Nitrogen-Sulfur-Carbon Materials for CO2 Reduction: Molecular Dynamics and Artificial Intelligence Study

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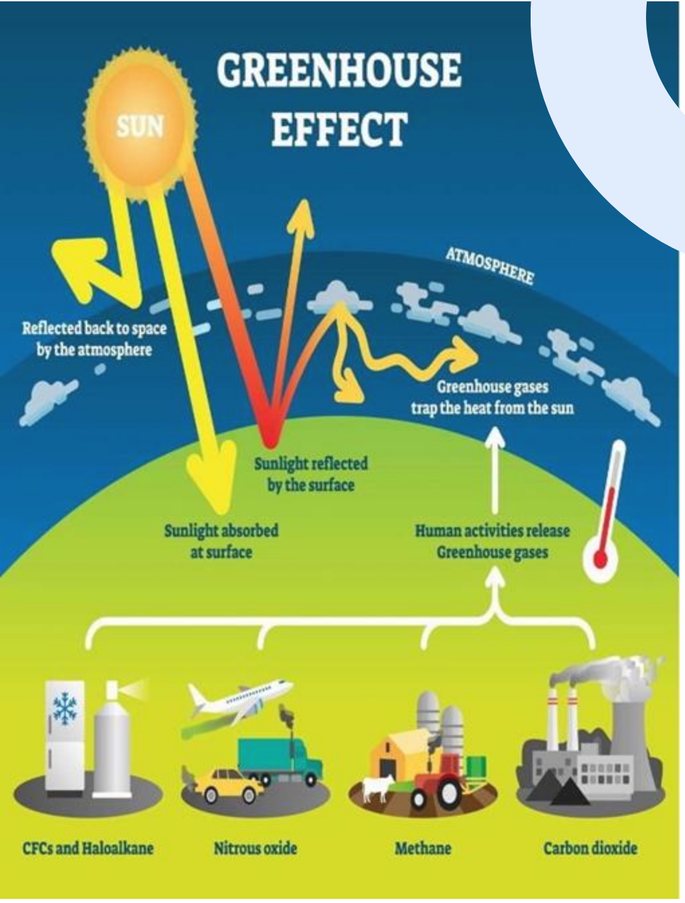


PURPOSE

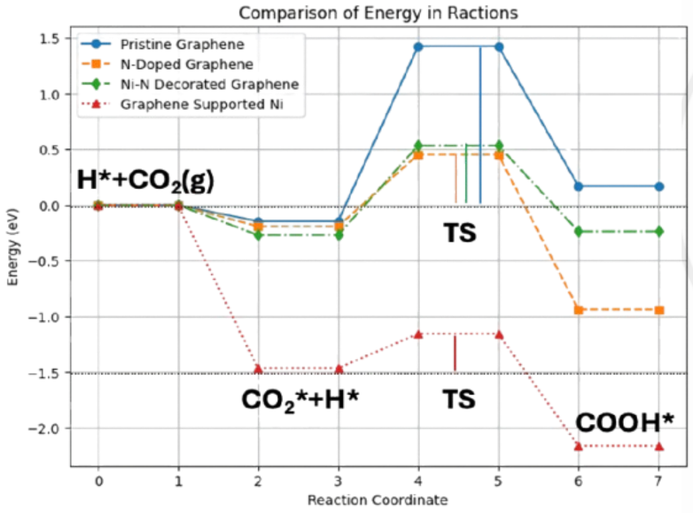
To design efficient nickel-based nano-catalysts on nitrogen-sulfur-carbon materials for CO_2 reduction using molecular dynamics simulations and artificial intelligence methods

OUTLINE

We investigate the catalytic activity of Ni cluster on Nitrogen-Sulfur-Carbon 2D material for CO_2 reduction into higher hydrocarbon products and methane

RESULT

DFT-assisted MD simulations revealed that Ni nanoparticles exhibited strong interfacial binding with the nitrogen-sulfur-carbon materials, which can serve as an effective catalyst for the CO_2 reduction



Computing system : SQUID General Purpose CPU Nodes
Node-hour : 1,000
Memory used : 64 GB
Parallelize: 10 nodes