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Atomic and molecular adsorption on Ni(111)

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Highlights

- Calculated binding structures and energies of atoms, molecules, and molecular fragments on Ni(111)
- Calculated vibrational frequencies of adsorbates on Ni(111)
- Estimated diffusion paths and barriers for adsorbates on Ni(111)
- Evaluated thermochemistry for the decomposition of NO, CO, NH₃, N₂, and CH₄ on Ni(111)

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