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First-Principles Study of the Products of CO₂ Dissociation on Nickel-Based Alloys: Trends in Energetics with Alloying Element

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Highlights

- Ni alloyed with metals in groups ≤ 6 bind atomic O stronger than alloy groups ≥ 7
- Atomic C binds stronger to the (100) than (111) facet of Ni-based alloy surfaces
- Alloying of Ni surfaces has little effect on CO binding
- CO dissociation is more favorable than the Boudouard reaction on Ni-based alloys

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