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Effect of substrate relaxation on adsorption energies: The example of α -Fe₂O₃(0001) and Fe₃O₄(111)

Adam Kiejna, Tomasz Pabisiak

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Highlights

- The differences between adsorption energies on iron oxides are explained.
- Influence of the substrate relaxation effects on adsorption energies is analyzed.
- The notion of the experimentally measured desorption energy is clarified.
- A huge difference between the desorption of CO on the Fe1 and O3 terminations.

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