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Influence of water, dihydrogen and dioxygen on the Stability of the Cr_2O_3 surface: a first-principles investigation

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Highlights

- DFT study of O₂, H₂O and H₂ interaction with (0001) Cr₂O₃ surfaces.
- Water adsorption on chromia surface: hydrated surface vs fully hydroxylation one.
- Surface reduction by H₂ is not thermodynamically possible.

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