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Surface Phase Diagrams of Titanium in Oxygen, Nitrogen and Hydrogen Environments: A First Principles Analysis

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Highlights

- Energetically stable geometries are determined for various concentrations of oxygen, nitrogen and hydrogen .
- The phase stability diagrams are determined to investigate the stability of various oxide, nitride and hydride phases as a function of finite temperature and gas partial pressure
- The evolution of spin polarization for all adsorbed cases are described

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