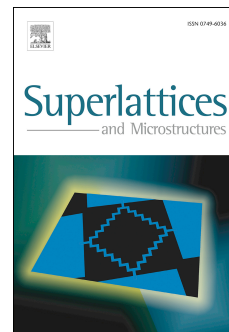


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# First-principles study of W, N, and O adsorption on TiB<sub>2</sub>(0001) surface with disordered vacancies

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## Abstract

In this paper, we systematically investigate the adsorption properties, atomic structures, electronic, and thermodynamic properties of tungsten, nitrogen, and oxygen atoms on the Ti-terminated TiB<sub>2</sub>(0001) surface without and with vacancies of titanium and boron atoms using the density functional theory (DFT). Local atomic structures of the surfaces R/TiB<sub>2</sub>(0001)

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