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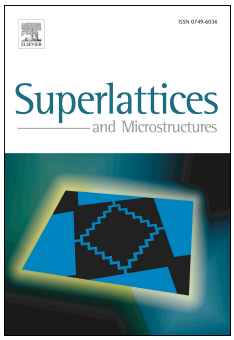

First-principles study of W, N, and O adsorption on TiB_2(0001) surface with disordered vacancies

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First-principles study of W, N, and O adsorption on $TiB_2(0001)$ 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 $TiB_2(0001)$ surface without and with vacancies of titanium and boron atoms using the density functional theory (DFT). Local atomic structures of the surfaces $R/TiB_2(0001)$