

Density functional theory study of anion ordering and chemical composition of different LaTiO₂N surface orientationsS. Ninova¹, U. Aschauer^{1*}¹University of Bern

Perovskite oxynitrides are a promising class of materials for photocatalytic water splitting under solar light.[1-3] They have the advantage of a reduced band gap with respect to the pure oxides, however at the cost of diminished stability. Perovskite oxynitrides are characterised by a partial order of oxygen and nitrogen atoms on the anion sublattice. In the bulk several theoretical studies find cis-positioning of the N-atoms to be energetically most favourable.[4-5] The anion ordering at the surface and its resulting chemical composition, however, are still elusive, despite its direct implication on the water-splitting mechanism on oxynitride surfaces.

We perform density-functional theory calculations on one member of the perovskite oxynitride class, LaTiO₂N, to deduce the O/N distribution for a variety of surface orientations and establish the chemical composition of the various surfaces and terminations. Based on these results it is possible to deduce trends for the reactivity of different surface orientations, which we correlate with experimental results on thin films with different orientations.

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