

Vortragsankündigung

Mittwoch, 15. Mai 2019, 11.15 Uhr

Seminarraum I (JAK2AOG1.33), Jakob-Haringer-Straße 2a

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“Surface structure and reactivity of perovskite oxynitrides”

The anion composition and order in perovskite oxynitrides presents an additional degree of freedom compared to pure oxides to tune material properties. In this talk I will highlight, based on our density functional theory (DFT) calculations, how the anion order at the surface is affected by the oxynitride's cation composition [1,2] and how it can change during photo(electro)catalytic applications of these materials [3]. Given the reduced stability of oxynitrides compared to oxides, we also assess the catalytic activity on surfaces where dissolution has altered the surface structure and show that this can, in fact, enhance the catalytic activity [4]. Finally, I will highlight the potentials but also drawbacks of strain engineering oxynitrides and introduce oxysulfides as alternative mixed anion materials to address these issues [5, 6, 7]. These theoretical results provide important insights on the atomic scale mechanisms underlying the surface structure of these promising photoelectrode materials and how the catalytic performance is affected by surface alterations under application conditions.

- [1] S. Ninova, U. Aschauer, *Surface structure and anion order of the oxynitride LaTiO₂N*, **Journal of Materials Chemistry A**, 5, 11040–11046, (2017)
- [2] H. Ouhbi, U. Aschauer, *Water oxidation chemistry of oxynitrides and oxides: Comparing NaTaO₃ and SrTaO₂N*, **Surface Science**, 677, 258–263, (2018)
- [3] H. Ouhbi, U. Aschauer, *Nitrogen loss and oxygen evolution reaction activity of perovskite oxynitrides*, **arXiv preprint** 1904.03077, (2019)
- [4] N. Vonrüti, U. Aschauer, *The role of metastability in enhancing water-oxidation activity*, **arXiv preprint** 1807.08546, (2018)
- [5] N. Vonrüti, U. Aschauer, *Anion Order and Spontaneous Polarization in LaTiO₂N Oxynitride Thin Films*, **Phys. Rev. Lett.**, 120, 046001, (2018)
- [6] N. Vonrüti, U. Aschauer, *Epitaxial strain dependence of band gaps in perovskite oxynitrides compared to perovskite oxides*, **Physical Review Materials** 2, 105401, (2018)
- [7] N. Vonrüti, U. Aschauer, *Band-gap engineering in AB(O_xS_{1-x})₃ perovskite oxysulfides: A route to strongly polar materials for photocatalytic water splitting*, **arXiv preprint** 1902.10211, (2019)