IAP Seminar

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Tuesday, 6th July, 2021, 16:00 s.t.
TU Wien, Freihaus HS 6, Turm A (grün), 2.OG, Raumnummer: DA02K01
Wiedner Hauptstraße 8-10
The seminar will be also held as a Zoom Meeting
https://tuwien.zoom.us/j/96062751637?pwd=ZkRUWnlkUFFZb2pEdm55ZzFteTBNdz09
Meeting ID: 960 6275 1637
Passcode: 9ANd8XWj

Complex oxide surfaces studied at the atomic scale by non-contact AFM/STM and DFT

The majority of solid state matter naturally appears in the form of an oxide, which are highly stable in atmospheric conditions, and therefore constitute a vast research area on a broad range of their properties. I will present results obtained on two representative materials: The model binary oxide rutile TiO_2(110) and the prototypical perovskite oxide $SrTiO_3$(001) oxide. Both were studied at the atomic scale at low temperatures in ultrahigh vacuum using combined non-contact atomic force microscopy (nc-AFM) / scanning tunneling microscopy (STM) experimental setup, and the results were directly compared to density functional theory (DFT) theoretical modeling.

Rutile TiO_2(110) interacts with the small O_2 [1] and CO [2] gas molecules by altering its polaronic ground state. A bulk-terminated $SrTiO_3$(001) surface can be obtained only through ferroelectricity-assisted cleaving in ultrahigh vacuum [3,4], which proved as a promising physical system for further investigations. In addition to the underlying physics and chemistry that give rise to these phenomena, I will introduce the techniques and discuss recent advances in the applied experimental and theoretical methodologies.

[1] I. Sokolović, M. Reticcioli, *et al.* "*Resolving the adsorption of molecular O_2 on the rutile TiO_2(110) surface by noncontact atomic force microscopy.*" Proceedings of the National Academy of Sciences **117**, 14827 (2020)
[2] M. Reticcioli, I. Sokolović, *et al.* "*Interplay between adsorbates and polarons: CO on rutile TiO_2(110).*" Physical Review Letters **122**, 016805 (2019)
[3] I. Sokolović, M. Schmid, *et al.* "*Incipient ferroelectricity: A route towards bulk-terminated $SrTiO_3$.*" Physical Review Materials **3**, 034407 (2019)
[4] I. Sokolović, G. Franceschi, *et al.* "*Quest for a pristine unreconstructed $SrTiO_3$(001) surface: An atomically resolved study via noncontact atomic force microscopy.*" Physical Review B **103**, L241406 (2021)

All interested colleagues are welcome to this seminar lecture
(30 min. presentation followed by discussion).

Friedrich Aumayr
(LVA-Leiter)

Ulrike Diebold
(Seminar Chair)