Fritz-Haber-Institut der Max-Planck-Gesellschaft

Physikalische Chemie — Direktor: Prof. Dr. Martin Wolf

MAX-PLANCK-GESELLSCHAFT

Department Seminar:

Monday, April 23, 2019, at **10:00** a.m.;
— all are invited to meet at around 9:40 for a chat and coffee —

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Layer-by-layer growth of TiO_2 - anatase: evolution 2D/3D of the electron states

PC Seminar Room G2.06, Building G, Faradayweg 4 R. Ernstorfer

Abstract:

Titanium dioxide (TiO_2) is mainly present in nature as three different polymorphs: rutile, brookite and anatase. In particular, the latter is largely studied due to its promising future applications in several devices like memristors and solar cells, as well as implementations in spintronics and transparent conductive oxides. In this framework, the most important physical quantity is certainly conductivity: it is thus fundamental to analyze and control the electronic properties of anatase with a particular attention to the surface, which plays a remarkable role in the previous applications.

Being thermodinamically favoured at the nanometric scale, a controlled and functionalized growth of anatase thin films is achieved through the extremely versatile and accurate technique of Pulsed Laser Deposition (PLD), while in-situ synchrotron radiation photo-emission spectroscopy measurements allow the investigation of the surface electronic properties.

Anatase TiO_2 is an insulator, however, recent studies report the presence of a dispersive electronic state at Fermi level and a non-dispersive in-gap state: despite the tremendous research activity, the nature of these states, especially the dispersive one, is still debated. In particular, for the latter it is contradictorily reported both a three-dimensional and a purely two-dimensional nature. Thus, to try to clarify this discrepancy, the evolution of the dispersive state has been analyzed as a function of thin film thickness, trying to find a possible correlation with the out-of-plane direction (namely, perpendicular to the surface). A preliminary investigation of the state evolution as a function of external solicitations like epitaxial strain induced by the substrate and thermal annealing has also been perforemed, with the purpose of providing more information regarding its physical properties.

Anatase thin films deposition by means of PLD required an intense materials science activity and the optimization of a suitable growth protocol. Nevertheless, the samples turned out to be of excellent quality, both regarding the optimal structural and superficial properties: the films possess an unique crystal phase, a well long range order and a very low surface roughness. Finally, the use of synchrotron radiation allowed an accurate investigation of the electronic properties: in particular, the dispersive state at Fermi level presents a quasi-two-dimensional nature, because its filling with electrons is correlated with the film thickness, while its response as a function of epitaxial strain and thermal annealing suggests a potential tunability behaviour controllable by appropriate external solicitations.