Open PhD-position

As part of the recently launched **FWF-funded project "Longer Acenes: Synthesis, Interface Formation, and Thin Film Stability"**, a PhD position is available in the "*Surface and Interface Science Group*" at the Institute of Physics, University of Graz. This interdisciplinary project is a collaboration between the experimental surface science and ab-initio electronic structure theory groups at the University of Graz, as well as the Institute of Organic Chemistry and the Institute of Physical and Theoretical Chemistry at the University of Tübingen, Germany.

About the project:

The project focuses on investigating the growth, stability, and electronic structure of longer acenes, a class of organic semiconductors, using advanced experimental and theoretical techniques. A key method employed will be photoemission orbital tomography, an innovative extension of angle-resolved ultraviolet photoemission spectroscopy (ARPES). These experiments will primarily be conducted using our state-of-the-art ARPES detector for 2D momentum mapping, as well as at European synchrotron radiation facilities. Additionally, low-temperature scanning tunneling microscopy (STM) will be used to gain molecular-level insights. The experimental work will be complemented by quantum-mechanical ab-initio calculations within the framework of (time-dependent) density functional theory. Exchange visits with our German project partners are an integral part of the collaboration.

Required qualifications:

We are seeking motivated candidates with the following qualifications:

- A Master's or Diploma degree in Physics.
- A strong interest in working collaboratively on cutting-edge surface science research.
- Technical skills and hands-on experience in experimental physics.
- Solid knowledge of solid-state physics.
- Familiarity with vacuum technology is highly desirable.

For detailed information please contact:

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Exploring Longer Acenes: Unlocking New Possibilities in Organic Electronics

Acenes, a class of hydrocarbons with linearly fused benzene rings, are key to organic electronics. Molecules like pentacene (five benzene rings) are widely used in transistors and solar cells. Beyond applications, acenes interest researchers in nanoscience, theoretical chemistry, and physics, where they are seen as one-dimensional analogs of graphene or carbon nanotubes. Longer acenes, such as hexacene, heptacene, and octacene, hold promise as high-performance organic semiconductors due to their exceptional electronic properties. However, their high reactivity and instability pose challenges for synthesis and application.

This collaborative project between the University of Graz (Austria) and the University of Tübingen (Germany) focuses on synthesizing and studying longer acenes, from hexacene to octacene. The aim is to systematically investigate their growth, structure, and electronic properties, from individual molecules to thin films. To address their reactivity, new fluorinated derivatives will be developed to enhance stability. These efforts will assess the feasibility of using longer acenes and their derivatives in organic electronic devices.

The project employs advanced experimental and theoretical techniques. Scanning tunneling microscopy (STM) will visualize individual molecules at the atomic level by measuring electron tunneling between a sharp tip and a surface. Photoemission orbital tomography (POT), based on angle-resolved photoemission spectroscopy, will provide insights into electronic structure, molecular orbitals, and adsorption geometry. POT involves irradiating a surface with monochromatic photons and analyzing emitted photoelectrons, offering a powerful tool for understanding molecular interactions.

Theoretical ab-initio density functional theory (DFT) calculations will simulate the electronic structure of acenes, complementing experimental data by predicting orbital-projected density of states, STM images, and photoemission angular distributions.

This interdisciplinary project unites experts in chemistry, physics, and materials science. The chemical synthesis of acenes and their fluorinated derivatives will be conducted by Prof. Bettinger's group at the University of Tübingen. Experimental studies will be led by Prof. Koller (University of Graz) and Prof. Peisert (University of Tübingen), while theoretical modeling will be carried out by Prof. Puschnig's team at the University of Graz.

By tackling the challenges of synthesizing and stabilizing longer acenes, this project aims to unlock their potential as active materials in organic electronics. Success could lead to innovative devices with improved performance and stability, advancing the field of organic semiconductors.