Contribution ID: **361** Type: **Talk**

【226】Photoemission Tomography on the Time-Domain: Simulation of Photoelectron Spectroscopy from Time-Dependent Density Functional Theory

Wednesday, 1 September 2021 15:15 (15 minutes)

Angular-Resolved Photoelectron Spectroscopy (ARPES) can benefit greatly from theoretical simulations as the observed momentum-space signature of the electronic structure is often quite involved. With the recent developments in ultra-fast laser physics, ARPES is now being used to also investigate time-resolved phenomena, e.g. for excited-states (pump-probe experiments).

In this talk we show how real-time Time-Dependent Density Functional Theory can be used to simulate time-resolved ARPES. Accounting for dynamical processes directly is an advance over established methods and reproduces experimental findings such as circular dichroism in molecular monolayers or 2D systems. Furthermore, we present how this method can be used to directly observe excitations in the electronic structure in time.

Primary author: Mr KERN, Christian Simon (University of Graz)

Co-authors: Dr YANG, Xiaosheng (Forschungszentrum Jülich); Dr DE GIOVANNINI, Umberto (Max Planck Institute for the Structure and Dynamics of Matter Hamburg); Dr SUBACH, Sergey (Forschungszentrum Jülich); Prof. TAUTZ, Frank Stefan (Forschungszentrum Jülich); Prof. RUBIO, Angel (Max Planck Institute for the Structure and Dynamics of Matter Hamburg); Prof. PUSCHNIG, Peter (University of Graz)

Presenter: Mr KERN, Christian Simon (University of Graz)

Session Classification: Surfaces, Interfaces and Thin Films

Track Classification: Surfaces, Interfaces and Thin Films