# Graduate School Seminar

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INSTITUT FÜR PHYSIK

Talks in SS 2018

Traditio et Innovatio

Universität Rostock

**07th** June 2018, **15:00 s.t.**

Gilbert Grell

**AG Molecular Quantum Dynamics**

## Resonant Auger Emission in a Quantum Chemistry Framework: The Neon Atom

Photoelectron spectroscopy is a widely applied tool to probe the electronic structure of matter. The X-Ray energy range yields access to core excited and ionized states, the energies of which are element specific. The core holes are usually localized on single atoms and their lifetime is determined almost exclusively by the Auger decay. Hence, X-Ray photoelectron spectroscopy (XPES) provides a local and site-specific probe of the electronic structure of molecular systems. This makes it possible to study a plethora of effects. Resonant Auger emission spectroscopy (RAES), detecting the electron emission after a resonant core excitation in the X-ray energy range, complements the picture of the electronic structure. Studying Auger emission from a theoretical perspective is a complicated task since the Auger decay is a pure correlation effect and requires a scattering theory consistent treatment of bound and continuum many body states. The obtained Auger emission spectra are especially sensitive to the model for the continuum electron.
In this talk I will demonstrate how RAES can be modeled from a quantum chemical perspective and discuss the sensitivity of the Auger emission of the $\mathbf{1s^{-1}3p^{1}}$ core excited state of the Neon atom with respect to different levels of approximation regarding the continuum electron. A possible route to a simpler model for atomic systems and a discussion of perspectives for the molecular case will be shown in the outlook.

Talk: English
Slides: English

**Location:** Institute of Physics, Albert-Einstein-Str. 24, HS 1