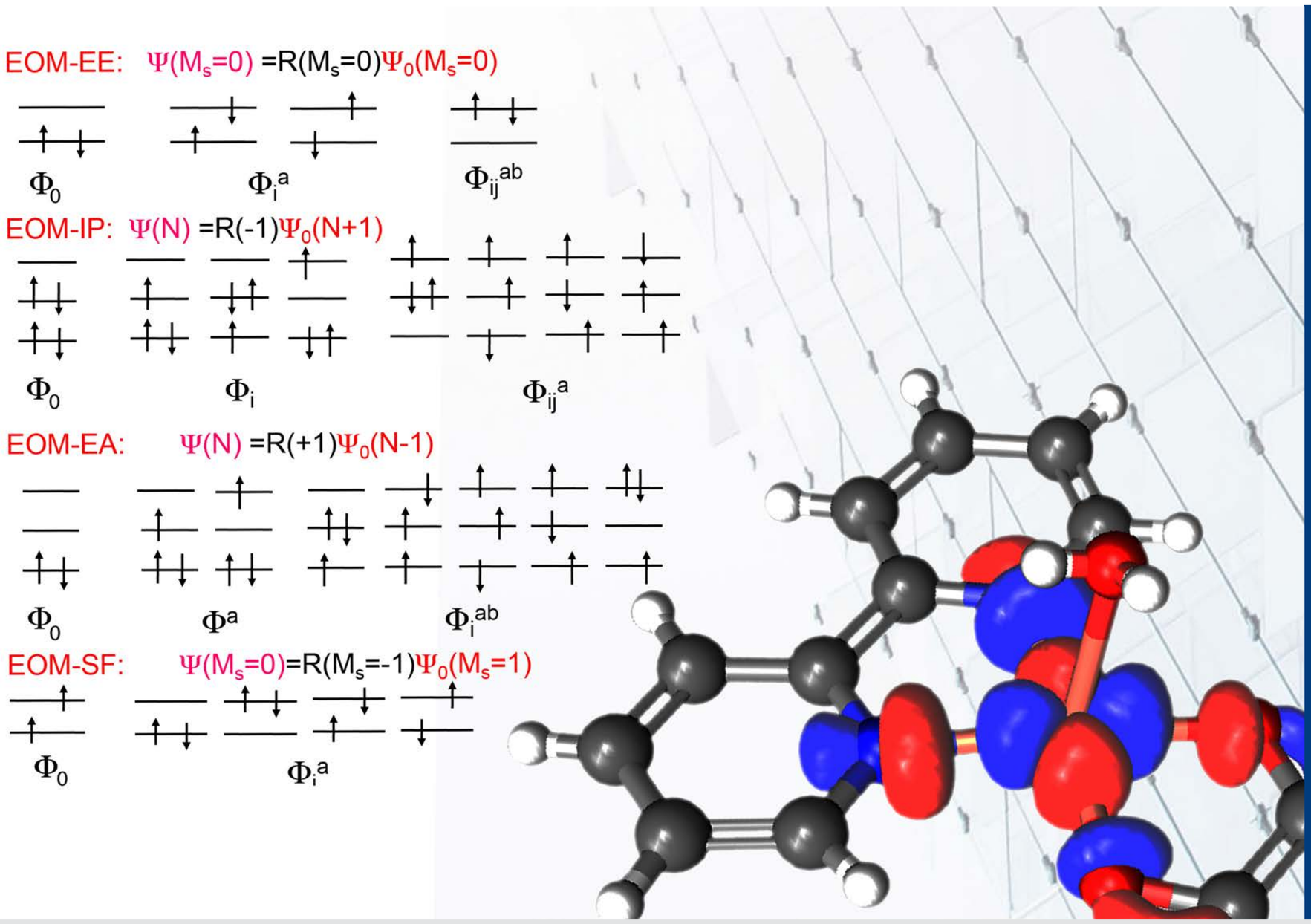
# MAINZ Master Class

# Quantum Chemistry of Bound Excited States and States in the Continuum

## Johannes Gutenberg University Mainz, June 24-25, 2019




## SPEAKERS

Anna I. Krylov (MAINZ Visiting Professor / University of Southern California, US)

Jürgen Gauss (Mainz)

Stella Stopkowicz (Mainz)

## CONTENT

The course will discuss advanced topics in quantum chemistry, focusing on electronically excited and open-shell species. The lectures will introduce methods for treating electronic correlation and bound excited states of isolated molecules. We will then discuss the concept of metastable states, illustrate their role in chemistry and physics by examples, and discuss their quantum-mechanical description, with an emphasis on practical approaches. Finally, we will discuss electronic structure of molecules perturbed by strong fields using magnetic fields as an example.

## TOPICS

- Electron Correlation and Coupled-Cluster Theory
- Equation-of-Motion Coupled-Cluster Theory for Electronically Excited States and Open-Shell Species
- States in the Continuum and Extensions of EOM-CC to Resonances via Non-Hermitian Quantum Mechanics
- Molecules in strong fields: EOM-CC Theory with Magnetic Fields (Perturbative and Non-Perturbative Regimes)

**PREREQUISITES**

Quantum mechanics and basic familiarity with quantum chemistry

PhD and Master students are welcome!

**VENUE** Helmholtz Institute Mainz, Staudingerweg 18, 55128 MAINZ

**REGISTRATION** https://mainz-quantum.eventbrite.de

**DEADLINE** June 17, 2019

**CONTACT** mainz@uni-mainz.de

**Registration: https://mainz-quantum.eventbrite.de**