



Post-doc position in computational materials science

A two-years postdoc position is available in the group of computational materials science at the department of Chemistry of the University of Zurich Switzerland ([Iannuzzi's group](#)) to work on the theoretical investigation of light induced processes and core level spectroscopy in condensed phase materials. Our group is interested in the development and application of computational methodologies for the atom-istic simulations of condensed matter. Our research is often strongly related to open questions on the fundamental understanding of physical and chemical properties and of the micro-structural evolution of complex systems of interest in technologically relevant fields. In this respect, our work is generally carried out in close collaboration with experimental partners and is focused on devising adequate models to address realistic aspects.

Your responsibilities: The successful candidate will work on the development and application of computational approaches to study light-induced processes at the nanoscale, by modelling the electronic structure beyond the ground state and addressing the role of excited states, non adiabatic dynamics, and charge transfer. The goal of the project is the assessment of general and flexible computational strategies to complement the recent advances in attosecond science, ultra-fast spectroscopies, and pump and probe experiments. The tasks are distributed among implementation, assessment of methods, and investigation of challenging phenomena induced by light-matter interaction. The combination of methods applied to complex systems, as liquids, nanostructures, and organic/inorganic interfaces, is going to be possible thanks to the integration into the high-performance computing infrastructure of the CP2K program package ([cp2k](#)), changing the perspective of feasible modelling and opening to a large number of possible applications.

Your Profile: We are looking for an experienced and motivated scientist, holding a PhD in Physics, Chemistry, or Materials Science. The applicants should have expertise in density functional theory and beyond-DFT methods for theoretical spectroscopy. Experience in modelling condensed matter systems is considered a valuable requisite. Excellent programming abilities (preferably in Python and Fortran) and strong records in theory and algorithmic developments are required and knowledge of high-performance computing is desirable.

What we offer: We offer a position in a stimulating work environment including the possibility to establish high-profile collaborations within the Swiss and international scientific network, as well as a competitive salary. The position is for two years, with extra funds available for traveling and collaborations. The city of Zurich offers a very dynamic and international living environment and is consistently ranked as one of the world's best city for quality of living by the Mercer survey.

Start of employment: The employment start date is by agreement. Interested applicants should send a cover letter, the CV, a research statement and names and email addresses of recommenders to marcella.iannuzzi@chem.uzh.ch Please submit your application as a single pdf.