Stellenanzeige

For our location in Hamburg we are seeking:

PostDoc in Electronic Structure Calculations & Nonlinear X-ray Science

Limited: 2 years | Starting date: 01.07.2021 | ID: FSPO010/2021 | Deadline: 07.06.2021 | Full-time

DESY, with its 2700 employees at its two locations in Hamburg and Zeuthen, is one of the world's leading research centres. Its research focuses on decoding the structure and function of matter, from the smallest particles of the universe to the building blocks of life. In this way, DESY contributes to solving the major questions and urgent challenges facing science, society and industry. With its ultramodern research infrastructure, its interdisciplinary research platforms and its international networks, DESY offers a highly attractive working environment in the fields of science, technology and administration as well as for the education of highly qualified young scientists.

Capabilities of modern X-ray sources such as X-ray free electron lasers open the possibility to transfer nonlinear optical techniques from the optical (visible) to the X-ray spectral domain. Within the DESY theory group on “Theory of Ultrafast X-Ray Science” we are developing novel X-ray spectroscopic and imaging techniques to unravel the electronic valence structure of solids. Within a combined experimental & theoretical effort we are currently investigating parametric nonlinear X-ray processes such as X-ray optical sum/difference frequency generation and X-ray parametric down conversion. These nonlinear processes promise to combine the spatial resolution of regular X-ray diffraction with spectroscopic selectivity, suitable to probe valence properties. Besides imprints of single-particle excitations within the band-structure, the method should allow characterization of collective excitations (plasmons) on atomistic scale. Recently, we have developed a theoretical framework based on non-relativistic quantum electrodynamics for describing X-ray optical wave mixing [1,2]. Currently, the underlying electronic quantities are based on density functional theory (DFT) calculations. The heart of this project lies in the improvement of the electronic structure calculations, by successive inclusion of correlation effects. Starting from different flavours of Kohn-Sham DFT and calculation of the electronic nonlinear response functions (density – current density correlation functions) the successful candidate will successively improve on the description of correlation effects, by application of (linear response) time-dependent DFT, random phase approximation and adiabatic-connection fluctuation-dissipation DFT and will explore the applicability of other methods, such as time-dependent current density functional theory. The theoretical results will directly tie in with the experimental activities of the group and external collaborators.

[1] C. Boemer, D. Krebs, A. Benediktovitch, E. Rossi, S. Huotari & N. Rohringer, Faraday Discussions, advance article, Jan. 6 (2021). Faraday Discussions, advance article, Jan. 6 (2021). Towards novel probes for valence charges via X-ray optical wave mixing https://doi.org/10.1039/D0FD00130A, http://arxiv.org/abs/2103.14710
[2] D. Krebs & N. Rohringer, submitted (2021). Theory of parametric X-ray optical wavemixing processes https://arxiv.org/abs/2104.05838

About the role:

The successful candidate will work in a team of theorists and experimentalists at the vivid research campus of DESY in Hamburg. The project will be carried out in a collaboration of the groups of Prof. Nina Rohringer (DESY & Universität Hamburg) and Dr. Mariana Rossi (Max Planck Institute for the Structure and Dynamics of Matter).

- Development of theoretical concepts and derivation of appropriate expressions for electronic current- density density correlators within the frame of several electronic structure theories of increasing complexity (DFT, linear response TDDFT, TD-CDFT, RPA, etc.)
- Software development: extension of existing electronic structure codes to implement the numerical calculation of electronic density – current density correlation functions
- Investigation of nonlinear response functions for a series of solids
- Strong interaction with experimental collaborators, application

To be successful in this role:

- PhD in the field of theoretical physics and theoretical material science or theoretical chemistry
- Strong background in electronic structure theory and/or computational physics
- Familiarity with the methods of DFT, (linear response) TDDFT and other, more specialised and advanced electronic structure methodologies would be an advantage
- Strong background in programming in C/C++ or FORTRAN
- Excellent communication skills in English and a strong interest in collaborating with collaborators on theory and experiment

For further information please contact Prof. Nina Rohringer +49 40 8998-6258 (nina.rohringer@desy.de).

We look forward to receiving your application via our application portal:

HELMHOLTZ
RESEARCH FOR GRAND CHALLENGES

Deutsches Elektronen-Synchrotron DESY
A Research Centre of the Helmholtz Association

of the theory to quantitative predictions for future experimental campaigns
- If interested, participation at experiments (beam times at X-ray free-electron lasers &electron storage-ring based X-ray sources)

Good reasons to join:

Look forward to a unique working environment on our international research campus. We attach particular importance to appreciative cooperation and the well-being of our DESY employees. You will benefit from our family-friendly and collegial atmosphere, our established health management and occupational pension provision. As a public employer, we offer you a secure workplace and facilitate your individual career with our comprehensive training and development opportunities. Remuneration according to the collective labour agreement (TV-AVH).

→ Apply now

DESY promotes the professional development of women and therefore strongly encourages women to apply for the position to be filled. In addition, severely handicapped persons with equal aptitude are given preferential consideration. The advertised positions are basically suitable for part-time employment.

You can find further information here:
https://www.desy.de/career/

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