

PhD scholarship in X-ray Tracking of Atomic Motion during Chemical Reactions using Free Electron Lasers

The [Centre for Molecular Movies](#) investigates ultrafast dynamic changes of inter- and intra-molecular structures during chemical reactions in solution. Our main tool is time-resolved X-ray scattering [1-2] in combination with complementary tools such as X-ray absorption spectroscopy [3]. Using these methods, we strive to understand the details of the interplay between electronic and structural degrees of freedom in chemical reactions, and through this understanding contribute to the development of new, functional materials for e.g. photo-catalysis and solar energy.

[Department of Physics at DTU](#) is now inviting applications for a PhD project under the headline of “X-ray Tracking of Atomic Motion during Chemical Reactions using Free Electron Lasers”. The PhD project will focus on optimizing the useful information that can be obtained from time-resolved scattering data. Inherent to the ultra-fast character of the experiments, the data contain significant contributions from laser-induced molecular anisotropy [4] as well as from X-ray beam coherence and a range of contributions closely linked to the interactions between molecules and solvent. This makes the data very information-rich, and at the same time very challenging to analyze. In the project we will investigate data inversion and modeling schemes as well as perform new cutting edge experiments at facilities for ultrafast x-ray science.

The successful candidate will be part of a dynamic and international scientific environment at the DTU Department of Physics and will work in close contact with our collaborators at [DTU Chemistry](#) and around the world. We have strong collaborations with leading groups in ultrafast x-ray science and photo-chemistry in Lund, Hamburg, Budapest, and Stanford, and a well-established track record at international x-ray sources for ultrafast science, notably the synchrotrons ESRF, and APS, and the free electron hard x-ray lasers LCLS and SACLA. We are closely connected with the European XFEL under construction in Hamburg, where we are contributing to the design and delivery of key components for the FXE (Femto-second X-ray Experiments) instrument in collaboration with the Danish company JJ X-Ray.

Qualifications

Applicants should have a master's degree in Physics, Chemistry, Engineering or similar. Experience with x-ray methods is a definite advantage. As the project will rely heavily on developing new software tools (Matlab) for data analysis in close connection with modeling (MD, DFT), experience with these tools and methods or a strong desire to acquire such skills is a must. The project will involve travel to international X-ray facilities for experiments a few times a year. As our projects are all of a highly collaborative nature, the candidate must have good person skills and have demonstrated the ability to work well within groups.

Approval and Enrolment

The scholarships for the PhD degree are subject to academic approval, and the candidates will be enrolled in one of the general degree programmes of DTU. For information about the general requirements for enrolment and the general planning of the scholarship studies, please see the [DTU PhD Guide](#).

We offer

We offer an interesting and challenging job in an international environment focusing on education, research, public-sector consultancy and innovation, which contribute to enhancing

the economy and improving social welfare. We strive for academic excellence, collegial respect and freedom tempered by responsibility. The Technical University of Denmark (DTU) is a leading technical university in northern Europe and benchmarks with the best universities in the world.

Salary and appointment terms

The salary and appointment terms are consistent with the current rules for PhD degree students. The period of employment is 3 years. Depending on seniority the salary level corresponds to around 40.000 EUR/yr.

Further information

Further information may be obtained from Professor **Martin Meedom Nielsen**, phone: +45 4525 3226, or email: mmee@fysik.dtu.dk (**Applications send to this address will not be considered; instead, please apply online as described below.**)

You can read more about DTU Department of Physics on www.fys.dtu.dk.

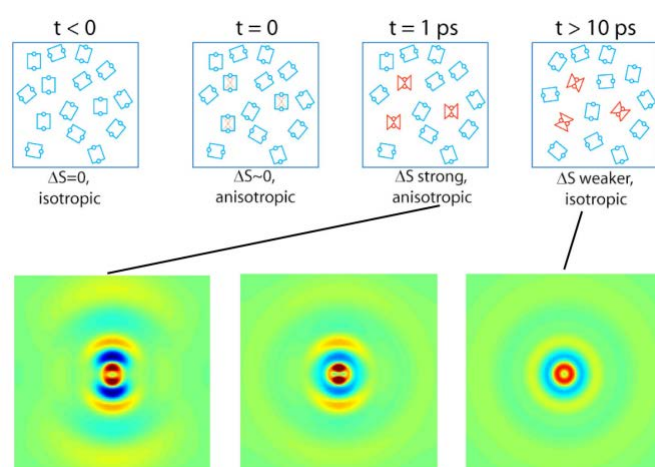
Application

We must have your online application by **May 6, 2013**. Apply online: www.tinyurl.com/cmm2013

Applications must be submitted as **one pdf file** containing all materials to be given consideration. To apply, please open the link "Apply online," fill in the online application form, and attach **all your materials in English in one pdf file**. The file must include:

- A letter motivating the application (cover letter)
- Curriculum Vitae
- Grade transcripts and BSc/MSc diploma
- Excel sheet with translation of grades to the Danish grading system (see guidelines and [excel spreadsheet here](#))

Candidates may apply prior to obtaining their master's degree, but cannot begin before having received it. All interested candidates irrespective of age, gender, race, disability, religion or ethnic background are encouraged to apply.



Anisotropic scattering patterns arising from orientation-dependent laser excitation of bimetallic molecules. The anisotropic images can be described by $\Delta S = S_0(Q) - P_2(\cos\theta_Q)S_2$, where S_0 and S_2 incorporate Bessel functions describing the structure of the molecule, P_2 is a 2nd order Legendre polynomial and the parameter θ_Q describes the geometry of the pump-probe experiment [4]. Significant new information can be obtained by analyzing the anisotropic rather than the isotropic images.