PHD POSITION IN THEORETICAL CHEMISTRY, AARHUS UNIVERSITY: The quantum description of two-photon absorption: Electronic, vibrational and solvent contributions

There is a phd position in theoretical chemistry associated with Ove Christiansen, Aarhus University. The general problem to be addressed is development and application of theoretical/ computational methods aimed at describing two-photon absorption.

Successful candidates are expected to have a strong background in Chemistry, Physics, Nano-science or similar, and have the ability and willingness to work with theory meaning both the basic equations, their realization in modern theories for electronic or nuclear degrees of freedom, programming and scientific computation. Qualifications beyond running standard programs is important.

On a daily basis the succesfull candidate will be included in the group of Ove Christiansen (www.chem.au.dk/~ove) There are long-lasting good relationships with several other groups in theoretical and computational chemistry creating an excellent common framework for courses, infrastructure (computers), general discussions, etc. The project and the project team is international from birth.

The chemical applications of the methods are related to the collaboration with experimental colleagues. All the above issues are important in connection with understanding and developing photo-sensitizers for producing singlet oxygen and applying reactive oxygen species for making oxygen based images, a research problem addressed in the interdisciplinary COMI center (Center for Oxygen Microscopy and Imaging, http://www.chem.au.dk/~comi/). The center for oxygen microscopy and imaging offers an excellent framework to learn from researchers in neighbooring disciplines. COMI is further connected to a EUROPEAN research Marie-Curie training network TOPBIO (http://ww2.icho.edu.pl/TOPBIO/) and the student is expected to participate in TOPBIO activities.

Relevant keywords: Theory, programming, Quantum Mechanics, ab initio electronic structure theory, vibrational structure theory, solvent effects, excited electronic states, photochemistry, one- and two-photon absorption, QM/MM or similar fragmentation methods, coupled cluster theory, molecular dynamics, C++, scientific computing, time-dependent quantum mechanics, response theory and molecular properties, anharmonic vibrational states.

Expressions of interest is forward to Ove Christiansen before June 15, 2011. Thereafter relevant applicants are short listed and contacted. This may include either online or real job interviews in Aarhus. Finally, a formal application is produced for acceptance into the Aarhus Graduate School Of Science (AGSOS).

An expression of interest should include: CV, list of publications, list of previous major projects, list of courses where the topics can be read, ECTS, list of grades, expression of research interests, motivation, programming experience, special qualifications, references, and possible starting dates. Please indicate where you first heard about the position.

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