

One post-doc position is available in the Department of Chemistry at the National University of Singapore, with expected starting period in the fall (October-November) or as soon as possible afterwards.

**Background and job description:**

Many interesting optic and magnetic properties of molecular systems involving transition metals and / or lanthanide ions are due to a combination of several factors: a) near-degenerate orbital ground state; b) strong spin-orbit coupling effects in the ground and excited states; and c) interactions between the electronic states with the available phonons in the molecular crystal (coupled atomic displacements). Theoretical predictions of optic and magnetic properties of such materials could be significantly enhanced if spin-orbit coupling and vibronic coupling are considered from first principles.

The current project will focus on developing a suitable, efficient computational scheme for the calculation of adiabatic and non-adiabatic vibronic couplings for transition metal / lanthanide compounds. The project will involve working with the existing computational packages and also developing and expanding the current possibilities of the employed code(s) for this particular class of materials. Applications of these developments would allow for higher level of trust for prediction of molecular geometries in ground and excited states, conical intersections between spin-orbit coupled states, estimation of magnetic relaxation of molecular magnets, optical properties of materials containing transition metals and /or lanthanide ions.

**Required skills & qualifications:**

- Knowledge of electronic structure methods, scientific programming and high-performance computing are highly welcome
- Expertise in scientific method and code development (Fortran / C or C++) in relation to one or several major quantum chemistry codes (e.g. MOLCAS, MOLPRO, DALTON, COLUMBUS, GAMESS, TURBOMOLE, ORCA, GAUSSIAN, VASP, or equivalent etc.);
- Scripting skills for automatization of workflow and data analysis
- Ability to work independently as well as in a team

The successful candidate is expected to hold (or be close to obtaining) an internationally recognized Ph.D. degree in quantum / computational chemistry, physics, applied mathematics, engineering, material science or closely related disciplines and an overall strong motivation.

**Work address:**

Department of Chemistry, National University of Singapore

**Job duration:**

The appointment will be initially for one year with possibility for extensions for an additional 2 years or longer depending on progress, performance and mutual agreement.

**Salary & Remuneration:**

Standard postdoc salary package ranges from S\$4500 to S\$5500 per month. Medical and leave benefits will be covered following the NUS standard rule.

Further information about this job please contact Dr. Liviu Ungur:

Email: [Ungur.Liviu@gmail.com](mailto:Ungur.Liviu@gmail.com)

**Application:**

Please send your CV, publication list and a letter of motivation to Mrs. Rachel Lucia Ng ([chmsec@nus.edu.sg](mailto:chmsec@nus.edu.sg)) and/or Dr. Liviu Ungur. Processing of applications will start on 1 July 2018 and continue until the position is filled.

Further information about the Department of Chemistry at NUS: <http://www.chemistry.nus.edu.sg>