Title: Quantum mechanical modelling of molecule-field interactions using RichMol

Molecule-field interactions are important to much current research in molecular physics and there is a growing demand for robust, theoretical approaches capable of simulating a variety of situations. RICHMOL is a new, general-purpose computer program for quantum mechanical modelling of molecule-field interactions. It is variational in its approach and treats all major electronic, nuclear motion, and external field effects. The program has been developed by Dr Andrey Yachmenev at the Center for Free-Electron Laser Science (CFEL) in Germany, but was originally started at University College London (UCL) in the UK.

RICHMOL utilizes the field-free, time-independent ro-vibrational energies and wavefunctions generated using the nuclear motion code TROVE [1, 2] (based at UCL). The time-dependent wavefunction is built from a superposition of field-free states and the time-dependent coefficients obtained by numerical solution of the time-dependent Schrödinger equation. The program can simulate electric fields of arbitrary strength, pulse shape and length. RICHMOL has already been used to propose a novel experiment for detecting chirality in linearly polarized fields [3].

The proposed short term scientific mission (STSM) has two main objectives: (i) to work on the publication of the methodology of RICHMOL so that the scientific community is aware that such a program exists (2 weeks), (ii) to use RICHMOL to start investigating new phenomena in polyatomic molecules such as induced chirality, optical centrifuge simulations, and non-linear field-induced ro-vibrational dynamics (2 weeks). The STSM will also provide an opportunity to discuss the latest developments in TROVE from the UCL side.

It is hoped that the STSM will help establish a long-term collaboration between the Controlled Molecule Imaging group at CFEL (predominantly experimentalists) and the ExoMol group at UCL (purely theorists). The planned work will contribute to the scientific goals of MOLIM's Working Group 1 (Energy-resolved methods) and Working Group 2 (Time-resolved method developments), notably in the area of laser control experiments.

References

[1] S. N. Yurchenko, W. Thiel, and P. Jensen, J. Mol. Spectrosc. **245**, 126 (2007).

[2] A. Yachmenev and S. N. Yurchenko, J. Chem. Phys. **143**, 014105 (2015).

[3] A. Yachmenev and S. N. Yurchenko, Phys. Rev. Lett. **117**, 033001 (2016).