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

The short term scientific mission (STSM) at the Center for Free-Electron Laser Science (CFEL) in Germany has been enjoyable and productive. As planned, significant progress was made on the RICHMOL methodology publication. It is hoped that this will be completed in the near future so that the scientific community is aware that such a program exists for quantum mechanical modelling of molecule-field interactions.

A new project on optical centrifuge simulations of polyatomic molecules was started. An optical centrifuge is a non-resonant laser pulse which undergoes accelerated rotation along the direction of propagation. The centrifuge field traps and forces the molecule to follow its rotating polarization. By gradually increasing the field's angular frequency, the molecule can be accelerated into extremely high rotational states. Accessing such states opens up interesting avenues of research in chemical dynamics.

Calculations were carried out on phosphine (PH_3) and ammonia (NH_3). These systems were chosen because they are examples of rigid and non-rigid molecules. Phosphine is a particularly interesting case as it forms rotational energy level clusters at highly excited rotational states. The resultant cluster states are chiral and an optical centrifuge is perhaps the most effective way to populate these states. Although there are still many open questions to address in this work, a good amount of progress was made on the project during the STSM. As a result, I was able to give a Molecular Physics seminar on optical centrifuge simulations of polyatomic molecules that was open to all groups at CFEL.

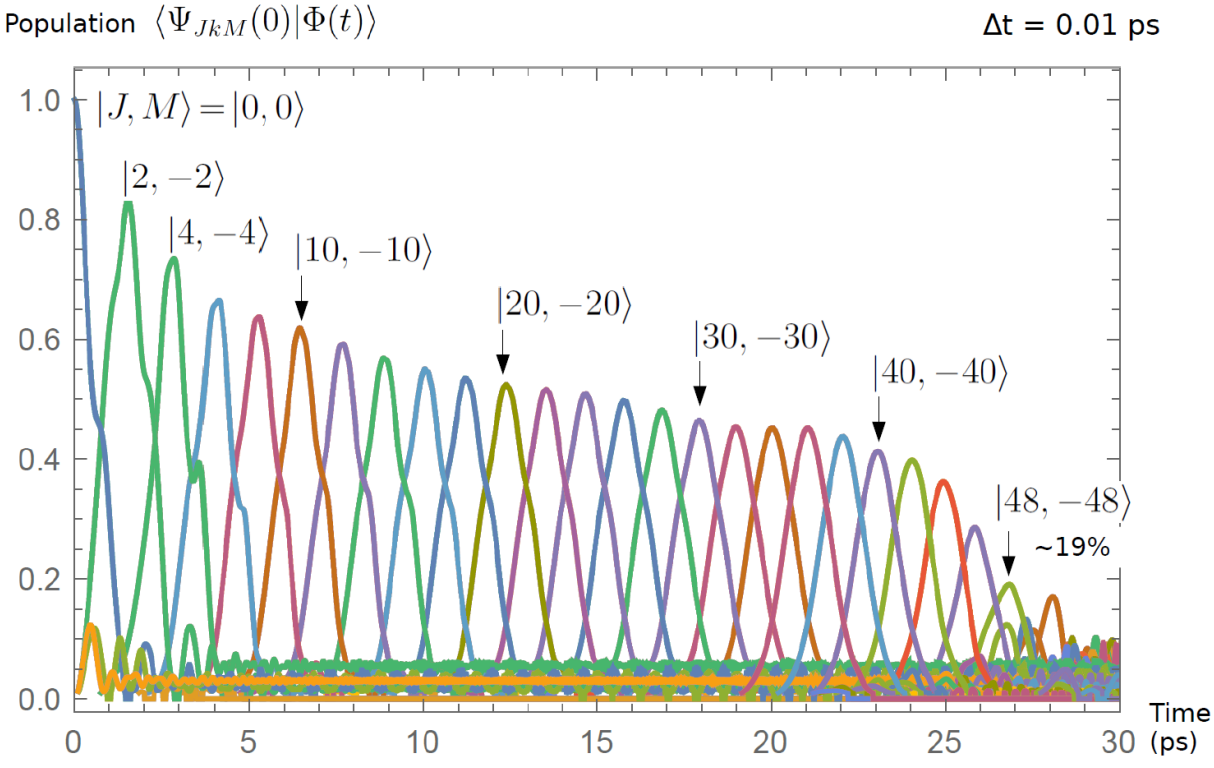

Figure 1: Climbing up the rotational ladder of PH_3.