Title:

Advancing molecular collision studies to the limits of first-principles quantum calculations and accurate spectroscopy; novel approaches for providing reference spectroscopic data for studying planetary atmospheres

The information about the atmospheres of Earth, other planets, their moons, and exoplanets are often obtained remotely by analyzing the light that passed through an atmosphere. The molecules that compose different atmospheric layers absorb light at specific frequencies leaving a fingerprint specific for a given molecular species. The problem can be reversed, and from analyzing a spectral structure of an overall absorption one can infer the atmospheric composition and properties such as pressure or temperature. An important factor in this methodology is that the structure (the shapes of optical molecular resonances) is perturbed by collisions between molecules. It is necessary to accurately describe these collisional effects to properly probe the atmospheres with remote spectroscopic techniques.

This project aims at a completely new approach to providing reference spectroscopic line-shape data based on experimentally validated ab initio quantum scattering calculations. On the one hand, we will perform the state-of-the-art numerical calculations of the collisional effects for molecular species that are relevant for atmospheric studies (such as O_2- and N_2-perturbed CO, O_2 and hydrogen halides). On the other hand, we will do complementary measurements based on ultra-accurate laser spectrometers with high-finesse optical cavities. A high-finesse optical cavity has a unique capability to circulate a laser beam for a long time with very small loss, which ensures exceptionally long light-molecule interaction time and hence a large sensitivity, which is critical for our studies. Finally, besides the atmospheric motivation, we will inverse the logic of the problem and instead of using quantum theory to provide useful reference spectroscopic data for various experiments, we will use our ultra-accurate measurements to validate the quantum calculations.