Quantum scattering of optically excited molecules

calculations from first principles and ultra-accurate measurements for molecular systems relevant for the studies of atmospheres of Earth, planets, and exoplanets

The main goal of this project is to use the extremely well controlled lasers to observe molecules. In particular we will use them to study fundamental physical and chemical properties, such as the structure of molecules, interactions between different atomic and molecular species and, most of all, the physics of the molecular collisions. At the molecular scale the collisions no longer can be treated classically, but should be rather viewed as full quantum phenomena of wave scattering. In practice, in our approach, the collisional effects can be observed as perturbations of the shapes of molecular optical resonances (in principle the laser-molecule interaction manifests as a series of sharp resonances; the presence of collisions make them broadened and result in a formation of sophisticated perturbations of their shapes). Within this project we will carry out both the theoretical calculations from first principles and collect the experimental data with a new extremely accurate laser technique. The goal of the project is to validate the quantum calculations on the highly accurate molecular spectra.

The collisional line-shape effects play an important role in atomic and molecular physics. As pointed out above, on one hand, they give an access to study the molecular interactions and dynamics but, on the other hand, they deteriorate accuracy of optical metrology based on molecular spectroscopy. In particular, the line-shape effects can limit the accuracy of atmospheric measurements of the Earth and other planets and even modify the opacity of the exoplanetary atmospheres. The reason for choosing this research topic is that we can use our quantum calculations and experimental advances to address this problem. We will use our experimentally validated quantum calculations to generate entire dataset of the line-shape parameters that can be used to improve the accuracy of the studies of the atmospheres of Earth and other planets, and exoplanets.

The theoretical part of our research will be mainly based on using the numerical methods to solve the relevant equations of quantum mechanics for the molecular systems important for atmospheric studies. We will use computer clusters (in our Institute and at the Institutes of our partners from other research groups) to perform the calculations. On the experimental side, we will use ultra-high-finesse optical cavities that are capable of storing the laser photons for a long time, which dramatically enhances the sensitivity and improves the accuracy of the method. Furthermore, we will implement a new approach (based on fast laser scanning) that will allow us to further improve the accuracy by at least one order of magnitude, which is pivotal for testing the collisional studies.