

## **Quantum scattering of optically excited oxygen molecules From fundamental physics to atmospheric research**

Within this project, we will use the basic laws of quantum theory to calculate how oxygen molecule collides with nitrogen molecules. Nitrogen and oxygen molecules are the main constituents of the Earth's atmosphere (nitrogen constitutes 78 % of the volume and oxygen 21 %), hence it is important to study the collisional effect for these two species. The most efficient way to collect the research data about the Earth's atmosphere is to use remote approaches based on molecular spectroscopy, which means that either the satellite missions or networks of ground-based platforms collect the light that passed through the atmosphere and perform detailed analysis of the light components that were absorbed by the molecules composing the atmosphere. The problem is that the spectroscopic signatures are largely perturbed by the fact that the molecules collide with each other very frequently at the atmospheric conditions. Therefore to accurately infer atmosphere properties (position dependent temperature, concentration and pressure) from the spectroscopic signals one need to have a very good understanding of the collisional processes. This project aims at solving this problem for the case of molecular oxygen. We will undertake detailed quantum calculations that will allow us to understand different collisional phenomena and provide reference data for atmospheric research. We will consider the A-band transitions – this band is well suited for the atmospheric research because the transitions from this band are sufficiently strong to be accurately recorded but not too strong to saturate the signal.

A second goal of the project is to use these calculations for fundamental studies. We will collaborate on it with the experimental group from the National Institute of Standards & Technology (NIST), Gaithersburg, USA. The combination of our fully quantum *ab initio* calculations of the collisional line-shape effects for the A-band molecular oxygen (that are planned within this proposal) and the complementary ultra-accurate experimental spectra from the NIST partner (acquired with the state-of-the-art cavity-enhanced techniques) will give us a unique opportunity to study physics of collisions at molecular scale.

These studies will be mainly based on using advanced numerical methods to solve the equations of quantum theory for describing molecular collisions. At the molecular scale the collisions no longer can be treated classically as we intuitively perceive it in every-day macroscopic experience, but should be rather viewed as a fully quantum phenomena of wave scattering. We will use the clusters of computer workstations (located at our Institute, the institutes of our partners from other research groups and public computing centers) to perform the calculations.