Tytuł projektu
Zderzenia atomów i molekuł w obecności spontanicznej emisji oraz autojonizacji
Project title
Collisions of cold atoms and molecules in presence of spontaneous emission or autoionization
Dyscyplina /Area of science
Nauki fizyczne
PROJECT DESCRIPTION

Motivation

The main objective of chemistry as a science is gaining the understanding of chemical reaction mechanisms and their optimal design. This is why understanding them at microscopic level, from `first principles' took a fundamentally important place in chemistry, as best proven by several Nobel prizes won by researchers in this and similar fields (in years 1986 Herschbach, Polanyi, Y.T. Lee, 1999, Zewail, and 2013 - Karplus, Warshel). The perfect practical realization of this dream is to conduct chemical reactions in perfectly controlled conditions. Cold chemistry was born only 20 years ago as a realization of the dream of attaining molecular Bose-Einstein condensate (BEC) and promised ultimate control of quantum dynamics experiments using highly controlled fields.
There are still unsolved puzzles how to tune the interaction between ultracold atoms and molecules or how to induce the chemical reactions between them. These puzzles are our main motivations.

Work Plan

First two years

- application of the close-coupling method with optical (complex) potential or other way of introducing losses (eg. boundary conditions). The method is essentially known but it was not studied systematically for optical potentials, nor for systems like highly excited atoms. The results can be confronted with finite grid methods such as DVR for bound states. Testing of the method will be performed on He*Li system (see next point) or existing data (potentials) for systems like Sr*Rb (group of Florian Schreck) or Yb*Yb (group of Takahashi).
- Penning ionization in magnetic field

  $He^* + A \rightarrow A^+ + He + e^-$

  We hope that using magnetic fields it will be possible to perform magnetic field-induced autoionization reactions. In Penning ionization the highest possible spin state of the He*A complex has the most stable character with lifetimes about 4 orders of magnitude longer than all the other spin states. We hypothesize that in systems consisting of the metastable helium atom and a paramagnetic molecule the Penning ionization can be suppressed in a controllable manner through the choice of magnetic fields and the reactant states. In the vicinity of Feshbach resonances, in turn, we should observe a sudden increase of the reaction rate of ion production due to the strong mixing of all spin quantum numbers of the whole complex. We will focus on two systems: first we will explore He*+Li system in collaboration with experimental group of Katrin Dulitz from University of Freiburg. Secondly, we will focus on the He*+O2 dimer for which we will also need realistic potential energy surface. The He*-O2 system will be our second-choice and it is possible to reschedule it to the second part of the project. Depending on circumstances collaboration with either Edvardas Narevicius (Weizmann Institute) or Andreas Osterwalder (EPFL) will be initiated.

Years 3-4 (might be subject to change depending on experimental needs and performance):

- studies of Hg+excited Hg collisions and Rb+excited Hg collisions. This part is particularly useful for experiments planned in FAMO laboratory in Torun. At the moment the ultracold mixture of Hg and Rb atoms was trapped, in near future experiments on optical Feshbach resonances and spectroscopy will start.
- as far as method development is concerned we will attempt to develop a new method based on (distorted wave) Born series which will allow to calculate the cross-sections as perturbation series, which will be far less expensive than regular close-coupling metod (N^2 scaling compared to N^3). The metod is somewhat similar to existing methods of Lowell Thomas (from 1980) which was never used for cold regime.

Required initial knowledge and skills of the PhD candidate: basics courses in molecular/atomic physics, quantum mechanics, or theoretical chemistry, basics in computer programming (preferably Python, Matlab), eager to learn

<table>
<tr><td colspan="2">Zgłaszający projekt/ Author of the project</td></tr>
<tr><td rowspan="2">dr hab. Piotr Żuchowski, prof. UMK

dr Mateusz Borkowski

stopień/tytuł, imię, nazwisko</td><td>pzuch@fizyka.umk.pl

mateusz@fizyka.umk.pl

e-mail</td></tr>
<tr><td>Instytut Fizyki UMK

jednostka organizacyjna</td></tr>
<tr><td colspan="2">Proponowani promotorzy i mentorzy/prospective supervisors</td></tr>
<tr><td colspan="2">1) promotor główny/ main supervisior</td></tr>
<tr><td rowspan="2">dr hab. Piotr Żuchowski, prof. UMK</td><td>e-mail : pzuch@fizyka.umk.pl</td></tr>
<tr><td>Instytut Fizyki UMK

jednostka organizacyjna</td></tr>
<tr><td colspan="2">2) promotor pomocniczy / co-supervisor</td></tr>
<tr><td colspan="2">Dr Mateusz Borkowski</td></tr>
</table>