

Popular summary of the project

„A diatomic molecule is a molecule with one atom too many” – Arthur L. Schawlow, Nobel Prize Laureate, 1980

The alkali metal dimers play a special role in studies of properties of diatomic molecules. In a simplistic view their theoretical description does not differ from that of H₂ molecule, the simplest of neutral diatomics – their properties are determined by two valence electrons. However, to get quantitatively correct results, also the remaining electrons and their mutual interactions have to be taken into account. This demands advanced theoretical methods. Alkali metal dimers are the optimum field to develop such methods – they are sufficiently complex so that the techniques used for description of more complicated molecules are also necessary for them, but at the same time sufficiently simple that numerical difficulties do not obscure essential physics of the problems.

Recently the alkali dimers have attracted additional attention in connection with development of laser cooling techniques. The alkali atoms were the first objects of cold physics experiments and they remain in the centre of attention of this field. At the same time, the first ultracold diatomic molecules were synthesized from alkali atoms by photoassociation and magnetoassociation (i.e. by using Feshbach resonances). A requirement for effective ways of detection of cold molecules and their transfer to the so called absolute ground state (i.e. with no electronic, vibrational or rotational excitation) brought about development of new experimental techniques like the stimulated Raman adiabatic passage (STIRAP) or resonance-enhanced multiphoton ionization (REMPI). Either for production or detection of cold molecules a precise knowledge of their electronic structure is necessary – both for the ground and the excited states.

Despite considerable progress in models and numerical methods of quantum chemistry, the most precise characterization of electronic states of alkali metal dimers originates still from experiments.

The scientific purpose of the project is experimental investigation of excited electronic states of alkali dimers Rb₂ and Cs₂. Several excited states in these molecules have been never observed and accuracy of the few existing theoretical calculations is far from precision attainable in the planned experiments. The investigations will be performed by a high resolution laser spectroscopy technique, the polarization labelling spectroscopy (PLS). In several cases this technique provides results unattainable with other methods. We plan that basing on measured energies of several thousands of rovibrational levels of Rb₂ and Cs₂ we shall construct potential energy curves characterizing various electronic states of the investigated molecules. Potential energy curves provide the best platform for comparison of theory and experiment. Confrontation of the experimental results with theoretical predictions is an important but not the main motivation of the project. Description of molecular states by potential curves constructed on the basis of experimental data is the most general one, as it allows to determine (by solving numerically a radial Schrödinger equation) all characteristics of a given state, like vibrational wave functions, energies of rovibrational levels, molecular constants, dissociation energy, rotational potentials etc. Such data are in particular essential for planning experiments on ultracold molecules. Our attention will be focused particularly on electronic states important for photoassociation and detection of ultracold molecules. The first goal will be investigation of these states, for which theoretical calculations predict potential energy curves with two minima but this has not been observed experimentally yet. Such a shape of the potential curve (in particular a presence of the second, broad potential well at large internuclear distances) makes these states good candidates for upper states in photoassociation process or intermediate states in various schemes of detection of ultracold molecules or their transfer to the absolute ground state. With sufficiently large experimental database the specialized numerical Pointwise Inverted Perturbation Approach method, developed in Warsaw, will allow us to construct highly precise potential energy curves of double minimum states allowing to reproduce energy structure of rovibrational levels with accuracy of order of 1 GHz. Such an accuracy is more than enough for verification of theoretical calculations for these states and, at the same time, facilitates a search of resonances in photoassociation experiments. It is worth noting that within the next few years experiments on formation of ultracold rubidium and cesium dimers are planned jointly at the Institute of Physics of the Polish Academy of Sciences and at the Faculty of Physics of the University of Warsaw.