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Excitation and emission spectroscopy of Rydberg states of diatomic van der Waals molecules containing 12. group elements

Abstract

The main goal of the presented thesis is a thorough understanding of the weakest interactions that bond atoms into bound states, i.e. van der Waals interactions (vdW). The thesis, as suggested by the title: *Excitation and emission spectroscopy of Rydberg states of diatomic van der Waals molecules containing 12. group elements* is divided into two parts: excitation and emission spectroscopy. The research is focused on Rydberg states of molecules which are defined by IUPAC as excited molecular states which are composed primarily of atomic orbitals with principal quantum numbers greater than that of the ground state [1]. In this work, only low-lying Rydberg states were investigated.

The first chapter provides information about the principles of van der Waals interactions, especially dispersive (London), and about the simplest objects containing such interactions – diatomic vdW molecules. Moreover, discrepancy between theoretically - and experimentally - resolved potential energy curves (PECs) in vdW molecules that leads to the ongoing enhancement of both theoretical and experimental tools is described. Naturally, the discrepancy is particularly marked in the case of Rydberg states. It is due to both: a large number of corrections that must be taken into account in *ab initio* calculations and the higher complexity of experimental design required to excite molecules to Rydberg states. This work focuses on the experimental determination of PECs of Rydberg states for diatomic vdW molecules.

The second, third, and fourth chapters contain a summary of research performed within the PhD thesis. Each of them begins with a short description of the contribution of the PhD student to published works. The second chapter contains results regarding excitation spectroscopy of CdRg molecules (Cd – cadmium atom, Rg - rare gas atom): isotopologue selection in optical – optical double resonance (OODR) method, characteristics of rotational profiles of the $\mathrm{E}^3\Sigma_1^+(6^3\mathrm{S}_1)$ Rydberg state of CdNe molecule, and experimental determination of a complete, double-well PEC of the $\mathrm{E}^3\Sigma_1^+(6^3\mathrm{S}_1)$ in CdAr including the shape of a potential barrier between two wells. The study of excitation spectroscopy is a main part of the presented thesis, and the experimental results were described in three articles being a part of the thesis: [2], [3], and [4].

In the third chapter a study on emission spectroscopy of Cd_2, CdRg, Zn_2 and ZnRg is described. An experiment that enables to record emission spectra from Rydberg states of vdW molecules was proposed and simulations of emission from ZnAr and CdAr Rydberg states were performed. The results were published in [5]. Furthermore, a theoretical model for an estimation of the number of excited molecules in OODR approach and

the number of detected photons was proposed in [6]. The calculations enable to predict whether emission spectra from newly-explored Rydberg states can be detectable.

In the fourth chapter the experimental study of Rydberg states of Zn_2 and ZnRg and its future prospective is described. A new source – module of molecular beam for zinc has been designed and built. A description of the source – module along with spectroscopic results of the $\mathrm{b}^3 0_\mathrm{u}^+(4^3\mathrm{P}_1) \leftarrow \mathrm{X}^1 0_\mathrm{g}^+(4^1\mathrm{S}_0)$ bound←bound excitation in Zn_2 were published in [7].

References:

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