Spectroscopy and Dynamics of Atomic Zinc Trapped in Xenon Matrices: Molecular Dynamics with Quantum Transitions

Hassiel Negrín-Yuvero, M. Lara-Moreno and G. Rojas-Lorenzo

Department of Atomic and Molecular Physics, InSTEC-University of Havana, Cuba

Experimentally, it is observed the emission and absorption bands -see figure 1- associated to the transition $^1S_0$-$^1P_1$, that take place in Zn atoms trapped in cryogenic matrices (Ne, Ar and Kr) upon the photoexcitation of the impurity [1]. In the particular case of Kr solids, it is also observed an emission band associated to $^3P_1$-$^1S_0$ transition [1]. This behaviuor has been studied for diatomic and triatomic complexes [2] and those studies shown the possibility to take place intercrossing amog $^1P_1$ and $^3P_2$ states, followed by intramultiple transitions $^3P_2$-$^3P_1$.

The picture is very different when the Zn atom is trapped in Xe matrices. Experimentally, there is not observe emission bands associated to the $^1P_1$-$^1S_0$ transition [1]. It means a high eficiency for intercrossing amog $^1P_1$ and $^3P_2$ states. In the experiments were recorded two bands red shifted respect to $^3P_1$-$^1S_0$ atomic emission. Similar picture was recorded when Cd atoms were photoexcited to their $^1P_1$ state, being trapped in Xe matrices []. But in this case one of the emission bands was associated to $^3P_1$ transition while the other one to the emission from the metastable state $^3P_0$.

The aim of the current work is concentrated on the study of the photoexcitation of atomic zinc trapped in Xe matrices. The study was carried out using the Molecular Dynamics with Quantum Transitions method. The Potential Energy Surfaces were built in the framework of the Diatomic in Molecule approximation. The results allowed to correlate the experimental data with the results obtained in the simulations during the photoexcitation of the impurity (see figure 2).

References

[1] V. A. Bracken, P. Gurtler, and J. G. McCaffrey, J. Chem. Phys., **107**, 5290, 1997

[2] J. G. Kaup and W. H. Breckenridge, J. Phys. Chem., **99**, 13701, 1995.

[3] J. G. Kaup and W. H. Breckenridge, J. Phys. Chem., **99**, 13701, 1995.

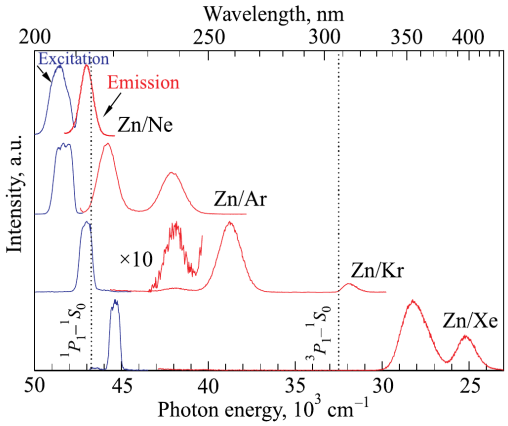

Figure 1. Experimental absortion and emission bands [1].

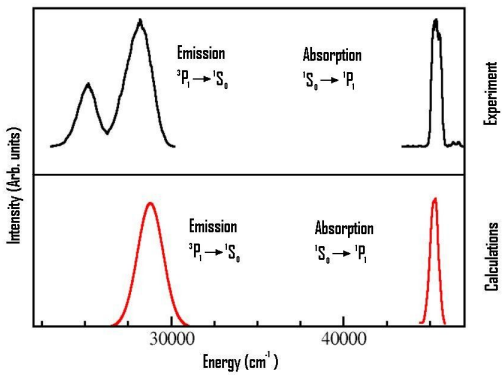

Figure 2. Experimenal [1] and calculated absorption and emission bands for Zn trapped in Xe matrices.