# Photoionization studies of some closed shell atoms and ions

A THESIS

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of

#### **DOCTOR OF PHILOSOPHY**



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THESIS CERTIFICATE

This is to certify that the thesis titled "Photoionization studies of some closed shell

atoms and ions", submitted by Sindhu K, to the Indian Institute of Technology, Mandi,

for the award of the degree of **Doctor of Philosophy**, is a bonafide record of the research

work done by him under my supervision. The contents of this thesis, in full or in parts,

have not been submitted to any other institute or university for the award of any degree

or diploma.

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# **Declaration by the Research Scholar**

I hereby declare that the entire work embodied in this thesis is the result of investigations carried out by me in the School of Basic Sciences, Indian Institute of Technology Mandi, under the supervision of Dr. Hari Varma and Prof P. C. Deshmukh, and that it has not been submitted elsewhere for any degree or diploma. In keeping with the general practice, due acknowledgments have been made wherever the work described is based on finding of other investigators.

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Date:	Signature:	
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#### **ABSTRACT**

KEYWORDS: Photoionization; many-electron correlations; relativistic effects; interchannel coupling; random phase approximation; Quantum Defect Theory; multi-configuration Tamm-Dancoff; cross-section; angular distribution parameter; Cooper minimum; configuration interaction; isonuclear; isoelectronic.

Study of interaction of electromagnetic radiation with the atom provides information about the atomic system. When a radiation of sufficiently high frequency is absorbed by an atom one or more electrons may be knocked out of the target, leaving the atom in an ionized state. These ejected electrons, known as photoelectrons, carry information about the atomic structure, electron-electron interactions and relativistic interactions present in the system.

In this thesis are reported the photoabsorption process of several closed shell elements including isonuclear and isoelectronic sequence using many body approximation methods Relativistic-Random-Phase Approximation (RRPA), Relativistic Multichannel Quantum Defect Theory (RMQDT) and Multi-configuration Tamm-Dancoff (MCTD). Photoionization cross sections and dipole angular distribution asymmetry parameters,  $\beta$ , of 5s and 4d shells of the closed-shell ions ( $La^{3+}$ ,  $La^{9+}$  and  $La^{11+}$ ) in the La isonuclear sequence have been studied using RRPA. The positions of the 5s Cooper minima in  $La^{3+}$  and  $La^{9+}$  ions are found to be extremely sensitive to the details of electron correlation. The results show that 5s cross sections of  $La^{3+}$  and  $La^{9+}$  do not lie along the same curve near the thresholds; the 4d cross sections, however, do match well in overlap regions so they lie along same curve, over the isonuclear sequence, except for a shift in threshold towards higher energies with increasing degree of ionization.

The autoionization resonances in the 5s cross section for  $La^{3+}$ ,  $La^{9+}$  and in the  $4d_{5/2}$  cross section for  $La^{11+}$  have been studied using RRPA and RMQDT techniques. The obtained resonance transitions are seen to be in the vicinity of extreme ultra violet region. Angular distribution asymmetric parameter  $(\beta_{5s})$  results for  $La^{3+}$ ,  $La^{9+}$  ions is

deviating from its non relativistic value 2.

The evolution of the 2s to np autoionization resonances for some of the members in the Mg isoelectronic sequence are reported using the RRPA+ RMQDT. The asymptotic quantum defects decrease monotonically with Z in the isoelectronic sequence. The angular momentum coupling scheme which is appropriate for the low-Z atom/ions is not the best suited for the high-Z ions, changing from Russell-Saunders to the jj scheme.

Photoionization studies of 5d and 6s subshells for atomic Hg using Multi-Configuration Tamm Dancoff method are also reported in the present work.

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