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Photoionization along the Cd Isonuclear Sequence

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ABSTRACT: Configuration-average distorted-wave calculations are carried out for the photoionization of Cd, Cd+, Cd^{2+}, Cd^{3+}, Cd^{4+}, Cd^{5+}, and Cd^{6+}. The first 4 ion stages have roughly the same peak cross sections, with a noticeable falloff for Cd^{4+}, Cd^{5+}, and Cd^{6+}. Photoionization cross sections for the Cd atom and its ions are needed to better understand planetary nebulae.

1. INTRODUCTION

Using the Immersion GRating INfrared Spectrometer (IGRINS) on the 2.7m telescope at McDonald Observatory, the Cd^{3+} emission line at 1.7204 micrometers was first seen in 2016[1]. The detection of this line provided new means to invesigate s-process nucleosynthesis in planetary nebulae progenitor stars. Photoionization cross sections for the Cd atom and its ions are needed to better understand planetary nebulae.

In this paper we carry out photoionization calculations for the first members of the Cd isonuclear sequence using an approximate configuration-average distorted-wave method[2]. The rest of the paper is structured as follows: in section 2 we review theory, in section 3 we present results, and in section 4 we give a brief summary. Unless otherwise stated, all quantities are given in atomic units.

2. THEORY

The photoionization of an atomic configuration has the general form:

$$(n_i l_i)^{w_i} \rightarrow (n_i l_i)^{w_i - 1} \epsilon_f l_f \ , \tag{1}$$

where n is the principal quantum number, l is the angular quantum number, w is the occupation number of the subshell, and $\epsilon = \frac{k^2}{2}$ is the electron energy. In Table 1 we list the $4d \rightarrow kl$ transitions for the Cd isonuclear sequence. Thus for Cd^{2+}, $n_i = 4$, $l_i = 2$, $w_i = 10$, and l_f = 1, 3 in Eq.(1).

In the dipole length gauge for the external electromagnetic field, the configuration-average photoionization cross section is given by:

$$\sigma_{ion} = \frac{8\pi\omega}{ck_f} \sum_{l_f} \frac{2w_i max(l_i, l_f)}{3(4l_i + 2)} \left[D(n_i l_i \rightarrow \epsilon_f l_f)\right]^2 \ , \tag{2}$$

where ω is the radiation field frequency and c is the speed of light. The radial dipole integral is given by:

$$D(n_i l_i \rightarrow \epsilon_f l_f) = \int_0^\infty dr P_{\epsilon_f l_f}(r) r P_{n_i l_i}(r) \ . \tag{3}$$

The energy and bound radial orbitals, $P_{nl}(r)$, are calculated in the Hartree-Fock relativistic (HFR) approximation[3]. The continuum radial orbitals, $P_{\epsilon l}(r)$, are calculated by solving a single channel radial Schrodinger equation, where the Hartree local exchange distorting potential is constructed with HFR bound orbitals and the continuum normalization is chosen as one times a sine function.

3. RESULTS

Configuration-average distorted-wave (CADW) calculations are carried out for the photoionization of Cd, Cd+, Cd^{2+}, Cd^{3+}, Cd^{4+}, Cd^{5+}, and Cd^{6+}. The cross sections from threshold to ω = 200 eV are presented in Figures 1-7.

The CADW cross sections for the Cd atom as presented in Figure 1 are found to have a peak cross section value around ω = 50 eV that is two times experiment[4]. On the other hand, many-body perturbation theory (MBPT) cross sections for the Cd atom[5] are in good agreement with experiment[4]. The MBPT cross sections include electron-electron correlation effects that are not included in the first-order perturbation theory CADW cross sections. However, as one moves along the isonuclear sequence to higher charged atomic ions, the nuclear attraction begins to dominate the screening effects due to electron-electron interactions. We also note that the photoionization cross sections begin to become much smaller after Cd^{3+}.

4. SUMMARY

Configuration-average distorted-wave theory has been applied to calculate photoionization cross sections for the Cd atom and Cd atomic ions from singly charged to six times charged. In the future we plan to calculate photoionization cross sections for moderately heavy atoms and their low charged atomic ions using a combination of non-perturbative close-coupling and perturbative distorted-wave methods.

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Table 1. Cd Isonuclear Sequence $4d \to kp, kf$ Transitions

Ion Stage	Initial Configuration	Ionization Potential
Cd	$4d^{10}5s^2$	17.50 eV
Cd+	$4d^{10}5s$	26.51 eV
Cd^{2+}	$4d^{10}$	36.69 eV
Cd^{3+}	$4d^9$	53.09 eV
Cd^{4+}	$4d^8$	70.61 eV
Cd^{5+}	$4d^7$	89.14 eV
Cd^{6+}	$4d^6$	108.61 eV

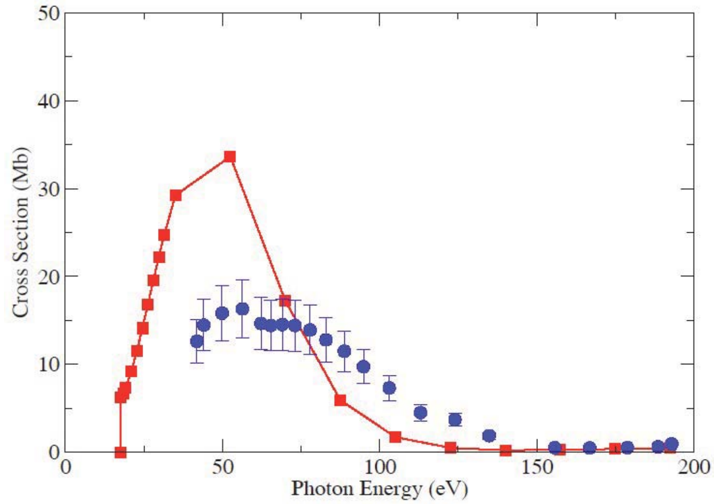

Figure 1. Photoionization of Cd. Solid line with squares (red) : $4d^{10}5s^2 \rightarrow 4d^9 5s^2 kl,$ Circles (blue) : experiment[4] (1.0 Mb = 1.0 × 10^{-18} cm^2).

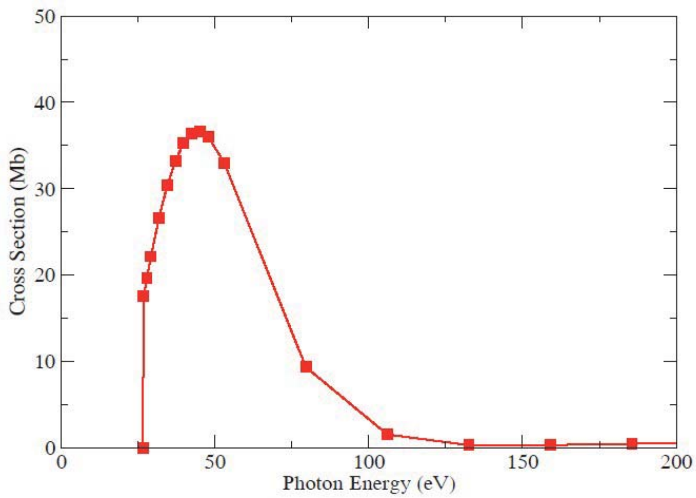

Figure 2. Photoionization of Cd^+. Solid line with squares (red) : $4d^{10}5s \rightarrow 4d^9 5skl$ (1.0 Mb = 1.0 × 10^{-18} cm^2).

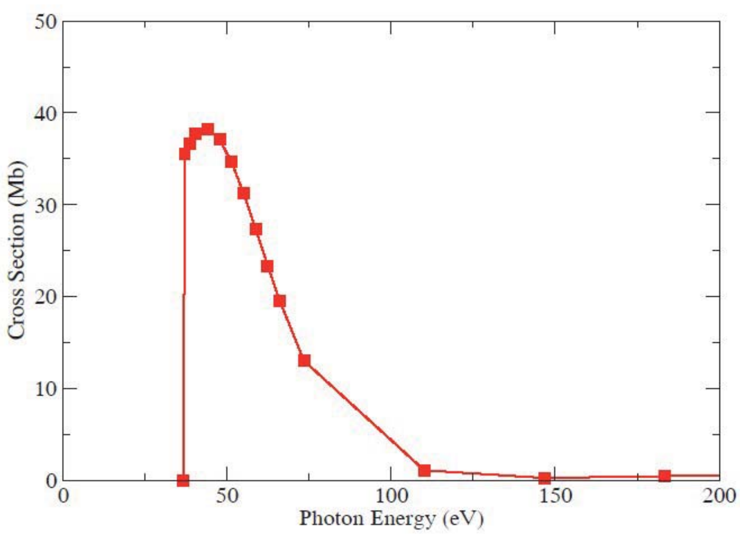

Figure 3. Photoionization of Cd^{2+}. Solid line with squares (red) : $4d^{10} \rightarrow 4d^9 kl$ (1.0 Mb = 1.0 × 10^{-18} cm^2).

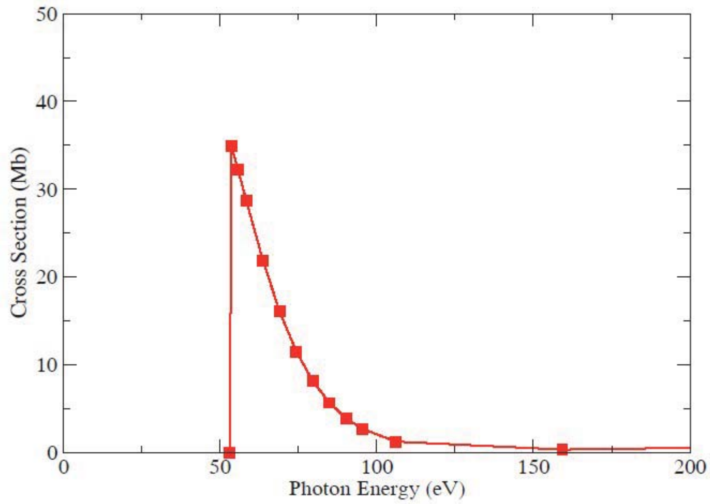

Figure 4. Photoionization of Cd^{3+}. Solid line with squares (red) : $4d^9 \rightarrow 4d^8 kl$ $(1.0$ **(1.0 Mb = 1.0 × 10^{-18} cm^2).**

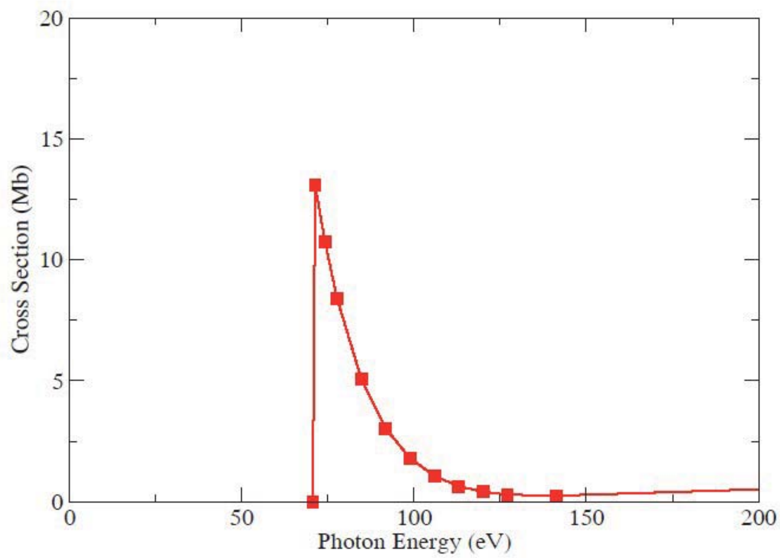

Figure 5. Photoionization of Cd^{4+}. Solid line with squares (red) : $4d^8 \rightarrow 4d^7 kl$ **(1.0 Mb = 1.0 × 10^{-18} cm^2).**

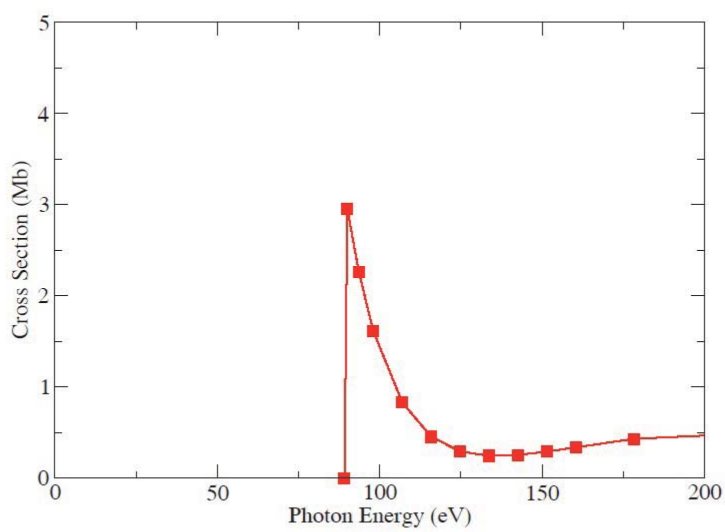

Figure 6. Photoionization of Cd^{5+}. Solid line with squares (red) : $4d^7 \rightarrow 4d^6 kl$ **(1.0 Mb = 1.0 × 10^{-18} cm^2).**

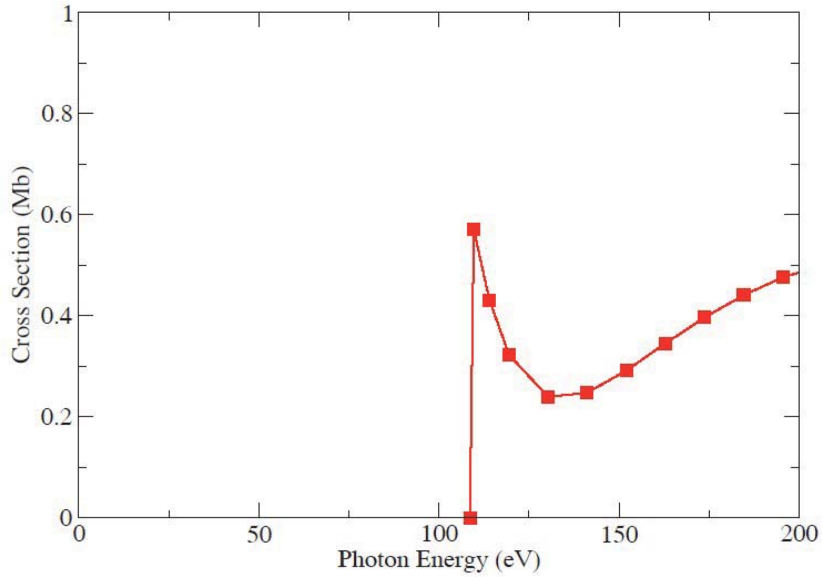

Figure 7. Photoionization of Cd^{6+}. Solid line with squares (red) : $4d^6 \rightarrow 4d^5 kl$ (1.0 Mb = 1.0 × 10^{-18} cm^2).