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Photoionization of Heavy Atoms and Ions

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ABSTRACT: A configuration-average distorted-wave method is used to calculate the photoionization cross sections for the Re, Os, Ir, Pt, and Au atoms, as well as their 1+, 2+, and 3+ ions. The bound atomic orbitals are found from Hartree-Fock relativistic calculations for the various heavy atoms and ions.

1. INTRODUCTION

In support of astrophysical observations of line radiation from heavy atoms and ions, we calculate the photoionization cross sections of the 5*d* block transition metals following tungsten. The elements Re, Os, Ir, Pt, and Au have large cross sections from the 5*d* subshell. These elements are believed to be generated efficiently in neutron star mergers[1]. The photoionized plasma environment near these kilonova events[2] means that accurate photoionization data for the low charge states of these elements is important for the interpretation of the spectra of neutron star mergers. The first neutron star merger was detected via gravitational waves and was accompanied by some spectral observations[2]. The determination of the abundances of the heavy elements made in the mergers is a key component in testing neutron star merger models.

The configuration-average approximation[3] has been found to be quite useful in calculating the photoionization of many atoms and molecules[4]. In this paper we carry out photoionization calculations for heavy atoms and ions using Hartree-Fock relativistic bound orbitals to generate the radial scattering potential for the continuum distorted-waves.

The rest of the paper is structured as follows: in section 2 we review the configuration-average distorted-wave (CADW) method for the photoionization of atoms, in section 3 we present CADW photoionization cross sections for Re, Os, Ir, Pt, and Au atoms and ions, 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:

$$(n_i l_i)^{\omega_i} \rightarrow (n_i l_i)^{\omega_i - 1} \in_f l_f \qquad (1)$$

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

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

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

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

The energy and bound radial orbitals, $P_{nl}(r)$, are calculated in the Hartree-Fock relativistic (HFR) approximation. 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

The CADW method is first used to calculate photoionization cross sections for the outer subshells of the Re atom ground configuration:

$$1s^2 2s^2 2p^6 3s^2 3p^6 3d^{10} 4s^2 4p^6 4d^{10} 4f^{14} 5s^2 5p^6 5d^5 6s^2 \tag{4}$$

The 6*s* orbital has an ionization potential of 7.93 eV and a peak cross section of 4.62 Mb just above threshold, the 5*d* orbital has an ionization potential of 9.44 eV and a peak cross section of 27.9 Mb at an incident photon energy of 18.9 eV, and the 5*p* orbital with an ionization potential of 55.33 eV has a peak cross section of 10.3 Mb just above threshold.

The CADW method is then used to calculate photoionization cross sections for the 5*d* orbital of the Re, Re^{+}, Re^{2+}, and Re^{3+} ground configurations. The ground configurations and the ionization potentials for the 5*d* orbitals are given in Table 1. The photoionization cross sections for the 5*d* orbitals are presented in Figure 1. The peak cross section for Re is 27.9 Mb at an incident photon energy of 18.9 eV, the peak cross section for Re^{+} is 31.0 Mb at an incident photon energy of 19.3 eV, the peak cross section for Re^{2+} is 28.5 Mb just above threshold, and the peak cross section for Re^{3+} is 14.4 Mb just above threshold.

Table 1. Re isonuclear Sequence 5d $\rightarrow kp$, kf Ionizations

Ion Stage	Initial Configuration	Ionization Potential
Re	$5d^5\ 6s^2$	9.44 eV
Re^{+}	$5d^5\ 6s$	17.53 eV
Re^{2+}	$5d^5$	26.50 eV
Re^{3+}	$5d^4$	38.97 eV

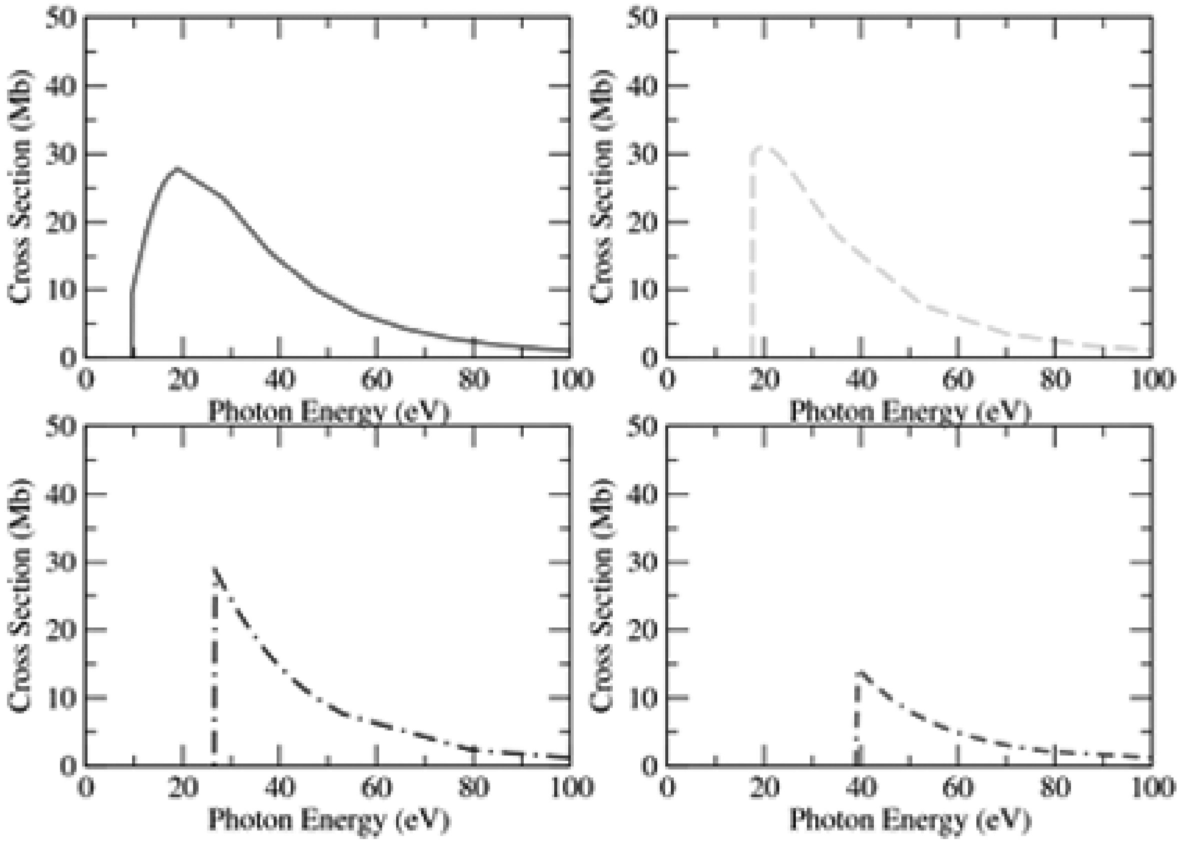

Figure 1. Photoionization of Re: $5d^5 6s^2 \longrightarrow 5d^4 6s^2 kl$, solid line, photoionization of Re$^+$: 5*d*56*s* $\longrightarrow$ 5*d*46*skl*, dashed line, photoionization of Re^{2+}: $5d^5 \longrightarrow 5d^4 kl$, dot dashed line, photoionization of Re^{3+}: $5d^4 \longrightarrow 5d^3 kl$, dot double dashed line (1.0 Mb = 1.0 × 10^{-18} cm2).

The CADW method is then used to calculate photoionization cross sections for the 5*d* orbital of the Os, Os^+, Os^{2+}, and Os^{3+} ground configurations. The ground configurations and the ionization potentials for the 5*d* orbitals are given in Table 2. The photoionization cross sections for the 5*d* orbitals are presented in Figure 2. The peak cross section for Os is 30.7 Mb at an incident photon energy of 21.0 eV, the peak cross section for Os^+ is 34.2 Mb at an incident photon energy of 22.7 eV, the peak cross section for Os^{2+} is 33.5 Mb just above threshold, and the peak cross section for Os^{3+} is 18.3 Mb just above threshold.

Table 2. Os Isonuclear Sequence 5d $\longrightarrow$ *kp*, *kf* Ionizations

Ion Stage	Initial Configuration	Ionization Potential
Os	$5d^6\ 6s^2$	10.51 eV
Os^+	$5d^6\ 6s$	18.88 eV
Os^{2+}	$5d^6$	28.13 eV
Os^{3+}	$5d^5$	41.00 eV

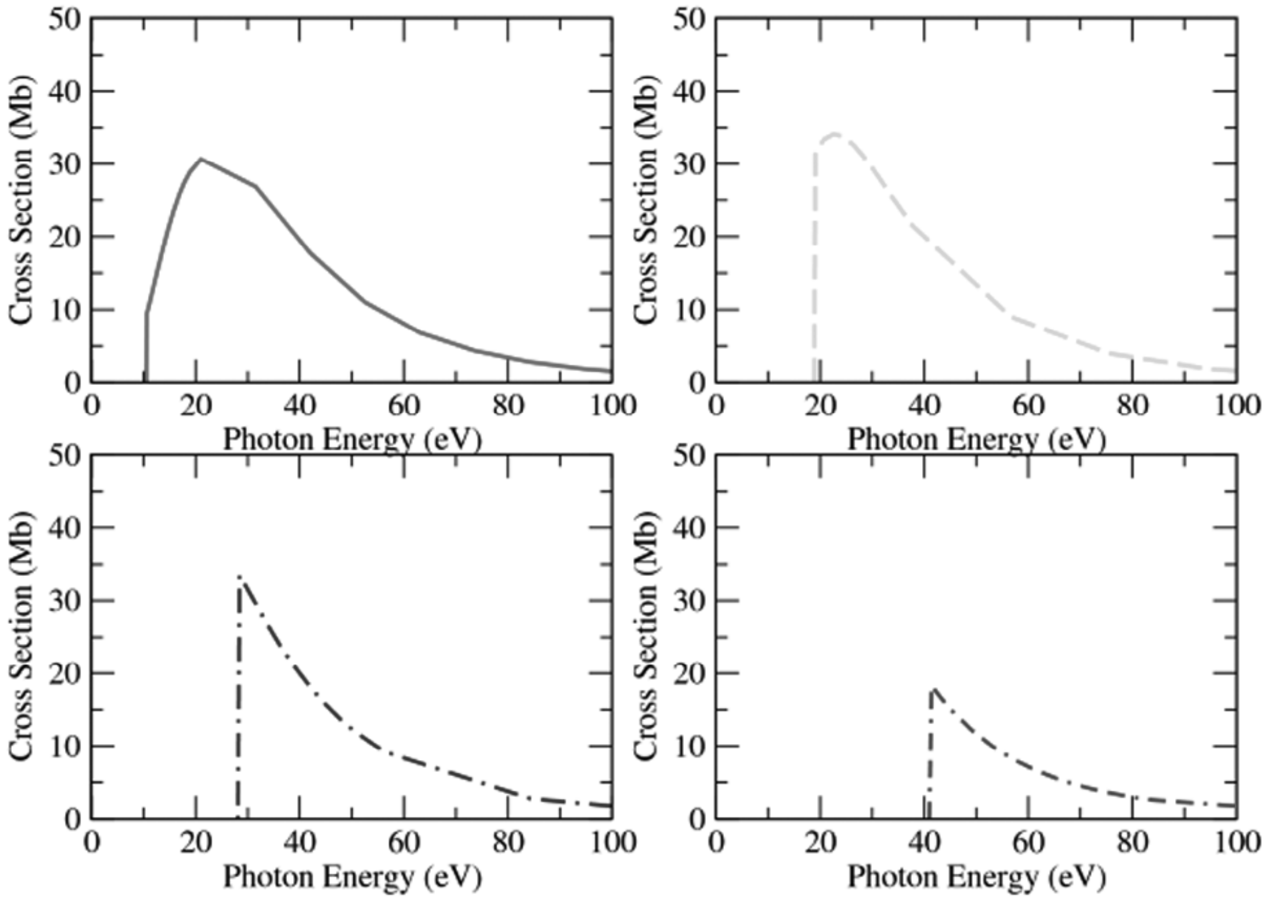

Figure 2. Photoionization of Os: $5d^6 6s^2 \rightarrow 5d^5 6s^2 kl$, solid line, pPhotoionization of Os^+: $5d^6 6s \rightarrow 5d^5 6skl$, dashed line, photoionization of Os^{2+}: $5d^6 \rightarrow 5d^5 kl$, dot dashed line, photoionization of Os^{3+}: $5d^5 \rightarrow 5d^4 kl$, dot double dashed line (1.0 Mb = 1.0×10^{-18} cm^2).

The CADW method is then used to calculate photoionization cross sections for the 5*d* orbital of the Ir, Ir^+, Ir^{2+}, and Ir^{3+} ground configurations. The ground configurations and the ionization potentials for the 5*d* orbitals are given in Table 3. The photoionization cross sections for the 5*d* orbitals are presented in Figure 3. The peak cross section for Ir is 33.0 Mb at an incident photon energy of 23.2 eV, the peak cross section for Ir^+ is 36.9 Mb at an incident photon energy of 26.3 eV, the peak cross section for Ir^{2+} is 38.0 Mb just above threshold, and the peak cross section for Ir^{3+} is 22.2 Mb just above threshold.

Table 3. Ir Isonuclear Sequence 5d → *kp*, *kf* Ionizations

Ion Stage	Initial Configuration	Ionization Potential
Ir	$5d^7$ 6s^2	11.60 eV
Ir^+	$5d^7\ 6s^2$	20.24 eV
Ir^{2+}	$5d^7$	29.77 eV
Ir^{3+}	$5d^6$	43.03 eV

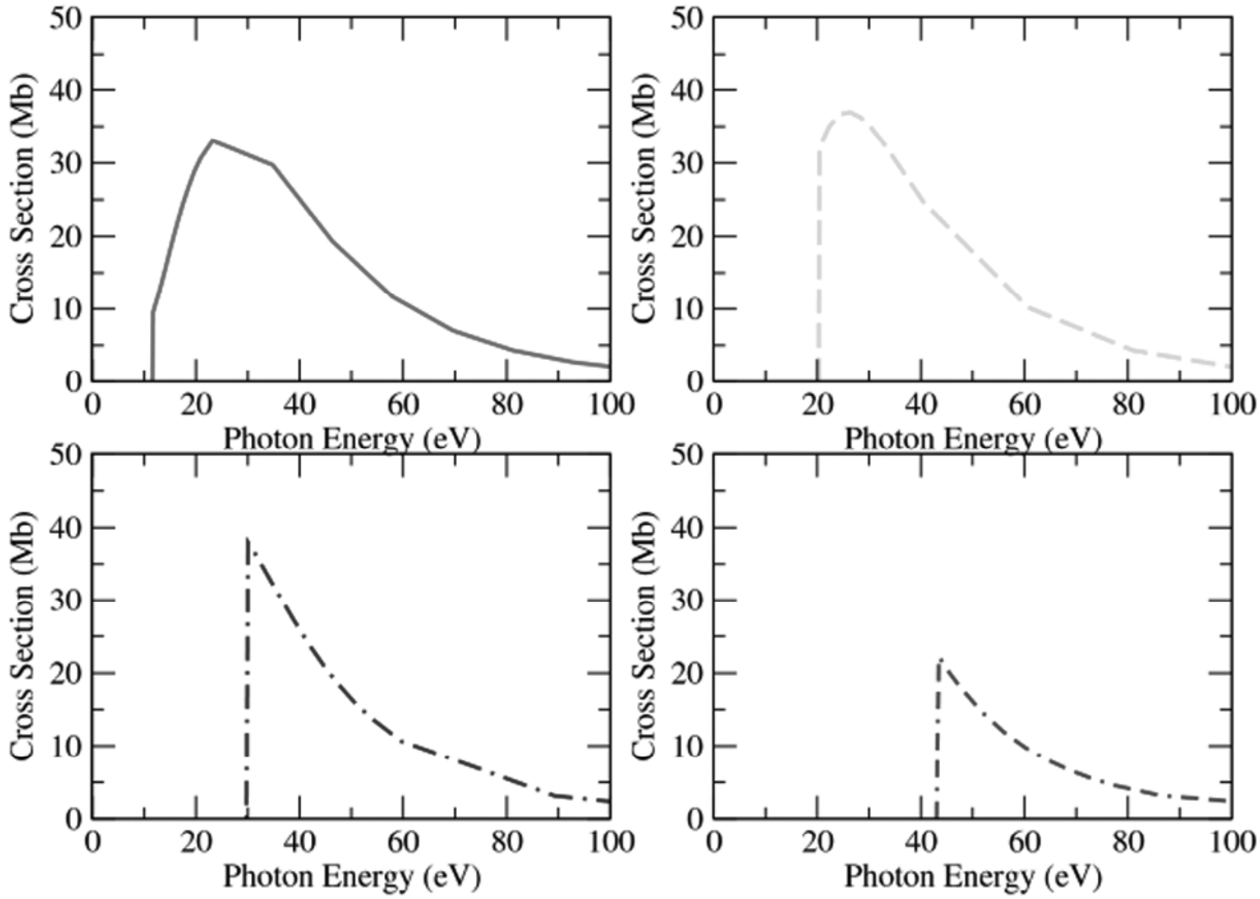

Figure 3. Photoionization of Ir: $5d^76s^2 \rightarrow 5d^66s^2kl$, solid line, photoionization of Ir$^+$: $5d^76s \rightarrow 5d^66skl$, dashed line, photoionization of Ir^{2+}: $5d^7 \rightarrow 5d^6kl$, dot dashed line, photoionization of Ir^{3+}: $5d^6 \rightarrow 5d^5kl$, dot double dashed line (1.0 Mb = 1.0 × 10 $^{-18}$ cm^2).

The CADW method is then used to calculate photoionization cross sections for the 5*d* orbital of the Pt, Pt$^+$, Pt^{2+}, and Pt^{3+} ground configurations. The ground configurations and the ionization potentials for the 5*d* orbitals are given in Table 4. The photoionization cross sections for the 5*d* orbitals are presented in Figure 4. The peak cross section for Pt is 38.1 Mb at an incident photon energy of 30.3 eV, the peak cross section for Pt$^+$ is 41.9 Mb at an incident photon energy of 26.4 eV, the peak cross section for Pt^{2+} is 41.8 Mb just above threshold, and the peak cross section for Pt^{3+} is 26.2 Mb just above threshold.

Table 4. Pt isonuclear Sequence 5d → *kp*, *kf* Ionizations

Ion Stage	Initial Configuration	Ionization Potential
Pt	$5d^9$ 6s	10.08 eV
Pt$^+$	$5d^9$	18.84 eV
Pt^{2+}	$5d^8$	31.40 eV
Pt^{3+}	$5d^7$	45.07 eV

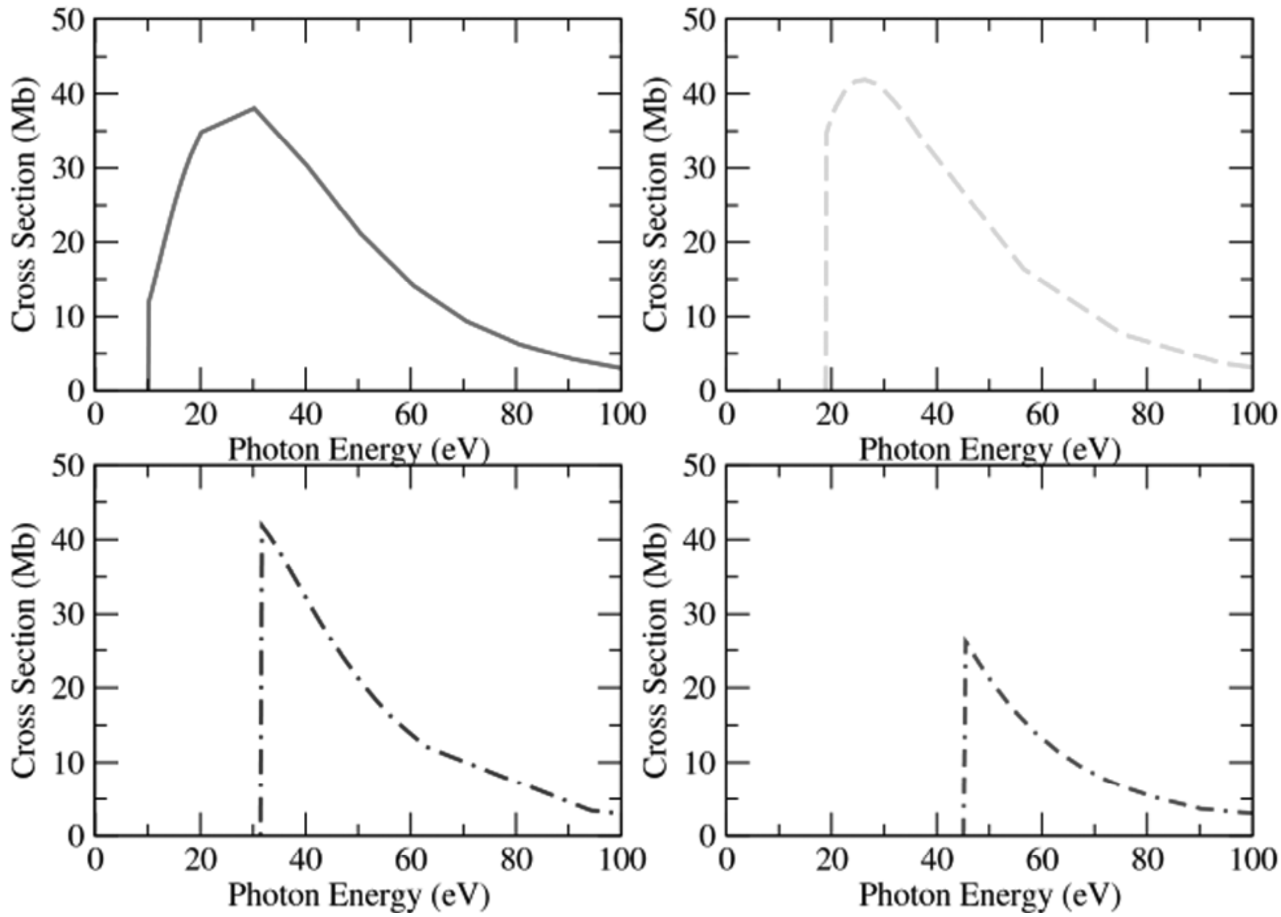

Figure 4. Photoionization of Pt: $5d^9 6s \rightarrow 5d^8 6skl$, solid line, photoionization of Pt^+: $5d^9 \rightarrow 5d^8 kl$, dashed line, photoionization of Pt^{2+}: $5d^8 \rightarrow 5d^7 kl$, dot dashed line, photoionization of Pt^{3+}: $5d^7 \rightarrow 5d^6 kl$, dot double dashed line (1.0 Mb = 1.0×10^{-18} cm^2).

The CADW method is then used to calculate photoionization cross sections for the 5*d* orbital of the Au, Au^+, Au^{2+}, and Au^{3+} ground configurations. The ground configurations and the ionization potentials for the 5*d* orbitals are given in Table 5. The photoionization cross sections for the 5*d* orbitals are presented in Figure 5. The peak cross section for Au is 40.2 Mb at an incident photon energy of 33.1 eV, the peak cross section for Au^+ is 43.6 Mb at an incident photon energy of 30.1 eV, the peak cross section for Au^{2+} is 45.1 Mb just above threshold, and the peak cross section for Au^{3+} is 30.2 Mb just above threshold.

Table 5. Au Isonuclear Sequence 5d → *kp*, *kf* Ionizations

Ion Stage	Initial Configuration	Ionization Potential
Au	$5d^{10}$ 6s	11.04 eV
Au^+	$5d^{10}$	20.07 eV
Au^{2+}	$5d^9$	33.05 eV
Au^{3+}	$5d^8$	47.11 eV

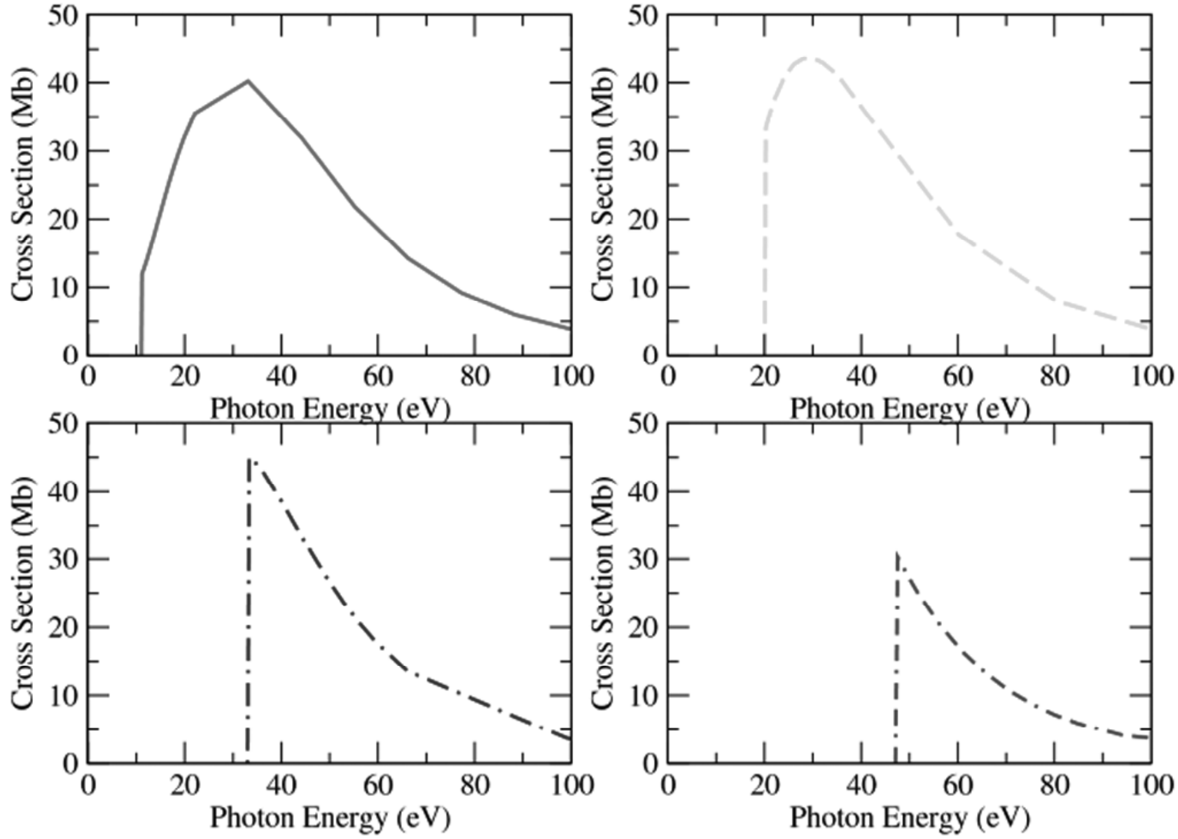

Figure 5. Photoionization of Au: $5d^{10}6s \rightarrow 5d^{9}6skl$, solid line, photoionization of Au^{+}: $5d^{10} \rightarrow 5d^{9}kl$, dashed line, photoionization of Au^{2+}: $5d^{9} \rightarrow 5d^{8}kl$, dot dashed line, photoionization of Au^{3+}: $5d^{8} \rightarrow 5d^{7}kl$, dot double dashed line (1.0 Mb = 1.0×10^{-18} cm^2).

4. SUMMARY

In conclusion, we have carried out configuration-average distorted-wave calculations for the photoionization of the Re, Os, Ir, Pt, and Au atoms, as well as their +1, +2, and +3 ions. In the future we plan to make furthur CADW calculations for photoionization of heavy atoms and ions. We plan to make detailed comparisons with current R-matrix calculations[5] for the photoionization along the Pt and Au isonuclear sequences.

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