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Ground-State Configurations and Unresolved Transition Arrays in Extreme Ultraviolet Spectra of Lanthanide Ions

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Abstract

Theoretical ground-state configurations of lanthanide ions calculated with the Cowan suite of codes are presented. Theoretical $4d - 4f$ and $4p - 4d$ spectra of Pd-like to Rb-like lanthanide ions calculated using the FAC relativistic code are also shown. The effects of configuration interaction are investigated and results compare favorably with experiments where, for increasing nuclear charge, strong emission peaks are observed to move towards shorter wavelength. The application of these strong emitters as extreme ultraviolet radiation sources, a topic of emerging interest, is discussed.

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I. INTRODUCTION

In 2003 Biemont and Quinet produced a comprehensive study of the structure and spectra of lanthanide atoms and ions [1]. They reviewed known experimental and theoretical spectra, transition probabilities, radiative lifetimes, hyperfine structures and isotope shifts. Currently ground configurations of the lanthanides are known experimentally for ion stages up to the third, and fourth in some cases [2]. As noted in [1], systematic analysis of spectra in higher ion stages of lanthanum and cerium have been performed: La VII [3], La VIII [4], La IX [5–8], La X [9], La XI [10, 11], La XIII [12], Ce III [13], Ce V [14], Ce VI [15], Ce IX [16], Ce X [17] and Ce XIV [10–12]. More recently progress has been made in analysing Cd-like ion spectra from Xe VII - Eu XVI [5, 18, 19] and Pd-like ion spectra [20].

In 1981 O’Sullivan and Carroll performed the first systematic recording of $4d - 4f$ emission in cesium through lutetium using the laser-produced plasma (LPP) technique [21]. The spectra displayed relatively narrow regions of resonance-like emission which became more complex and moved to shorter wavelength with increasing nuclear charge, Z . They attributed these emissions in a given element to $4d - 4f$ transitions overlapping from several adjacent ions. A complimentary work by the same authors [22] predicted the ground-state configurations from experimental results, of ions I through XVI for $Z = 57 - 74$. This aided the interpretation of $4d - 4f$ emission in the lanthanides and linked the complexity in the spectra to $4f$ electron occupancy in the ground state.

Since then, there has been much research done to understand the origin of these complicated spectra. Mandelbaum *et al* [23] used the unresolved transition array (UTA) model developed by Bauche-Arnoult, Bauche and Klapisch [24–27], and to account for configuration interaction (CI), carried out *ab initio* calculations on La to Eu using the relativistic RELAC code [28]. They concluded that interactions between the $4p^6 4d^{N-1} 4f$ and $4p^5 4d^{N+1}$ configurations are responsible for narrowing the transition arrays and their superposition in adjacent ion stages. This theory was supported by the recording of absolutely calibrated soft X-ray spectra from laser plasmas of various materials with atomic numbers ranging from 57 – 82 [29].

Motivation for this work arose from a number of factors: a natural theoretical follow on from Carroll and O’Sullivan’s earlier experimental work [22], techniques used for the analysis of gadolinium and terbium experimental spectra [30] can be applied to similar lanthanide

ions, search for a successor at shorter wavelengths to tin, xenon and lithium plasmas as a source for extreme ultraviolet (EUV) lithography, search for an XUV / soft X-ray source for metrology and use in microscopes for biological sampling, and finally to give a comprehensive overview of trends in theoretical atomic structure and spectra along the lanthanide series. In section II we present results of calculated ground-state configurations of Ag-like to Ho-like lanthanide ions. In section III we present 180 theoretical $4d - 4f$ and $4p - 4d$ unresolved transition array (UTA) spectra, for ions with configurations $4p^6 4d^N - 4p^6 4d^{N-1} 4f$ and $4p^6 4d^N - 4p^5 4d^{N+1}$, $N = 1..10$. Also in this section we discuss the effects of CI, and overall trends in the position and intensity of UTA peaks from La to Lu. Finally in section IV we conclude with a summary of this study of lanthanide ions.

II. GROUND-STATE CONFIGURATIONS OF LANTHANIDE IONS

As in [30, 31], *ab initio* calculations were performed using the Hartree-Fock with relativistic and correlation corrections mode of the Cowan suite of atomic codes [32] for the lanthanide ions. It is well known that the $4f$ binding energy increases more rapidly with increasing ionization than that of either the $5p$ or $5s$, which leads to significant reordering of configuration energies. All configurations considered from Ag-like to Ho-like ions are presented in Table I. In this table $M + N + K = 6$ means that configuration average energies of $5s^2 5p^4$, $5s^2 5p^3 4f$, $5s^2 5p^2 4f^2$, $5s^2 5p 4f^3$, $5s^2 4f^4$, $5s 5p^5$, $5s 5p^4 4f$, $5s 5p^3 4f^2$, $5s 5p^2 4f^3$, $5s 5p 4f^4$, $5s 4f^5$, $5p^6$, $5p^5 4f$, $5p^4 4f^2$, $5p^3 4f^3$, $5p^2 4f^4$, $5p 4f^5$ and $4f^6$ were calculated. The ground configuration was taken as the one with the lowest calculated average energy [33, 34] and these results are illustrated comprehensively in Fig. 1 and Table II.

As noted by Carroll and O’Sullivan [22], the behaviour of the $4f$ electron is crucial for an understanding of the ground-state configurations of the lanthanides in their various stages of ionization. The ground states for the neutrals and the first three ion stages are known experimentally [2] and are presented in Table I of [22]. In order to establish a trend in the ground-state configurations we look at the Xe-like sequence. Fig. 1 (c) highlights the position where a crossover from $5p$ to $4f$ occupancy in the ground-state configuration occurs. In the earlier work [22], it was proposed (based on experimental evidence) that the ground-state configuration was $5s^2 5p^6$ from La IV - Pr VI which is consistent with our current calculations. (Discrepancies between the current study and the previous work [22] are highlighted in

bold in Table II). Following this, it was expected that due to $4f$ -wavefunction collapse, whence the $4f$ electron becomes more tightly bound than the $5p$ electron, the ground-state configuration would be $5s^24f^6$ for Nd VII - Ho XIV as presented in Table I of [22]. Our calculations disagree from Nd VII - Eu X, where the ground-state configuration is found to be $5s^25p^6$ for Nd VII, $5s^25p^54f$ for Pm VIII, $5s^25p^34f^3$ for Sm IX, $5s^25p^24f^4$ for Eu X and $5s^24f^6$ for Gd XI. This would indicate that the best description is contraction rather than collapse and there is considerable interaction between the $5p$ and $4f$ orbitals until Gd XI. It was also predicted that the ground-state configuration for Er XV and Yb XVI would be $4d^{10}4f^8$. We calculated $5s^24d^{10}4f^6$ for Er XV and $5s4d^{10}4f^7$ for Yb XVI which again indicates an interplay of the $5s$ and $4f$ orbitals, at the 14^{th} ion stage in agreement with [22]. In [34, 35] the same sequence was calculated in a non-interacting regime using the Froese-Fischer [36] MCHF code. The results presented in Table I of [35] differ considerably in the order of filling of $5p$ versus $4f$ and $5s$ electron occupancy. We now consider the isoionic sequence of six times ionized ions. In [22] it was proposed that once the $4f$ crossing has occurred at Pr VII, the $4f$ shell will continue to fill until Er VII is reached with $5s^24f^{14}$, past which the ground-state configuration would be of the type $5s^24f^{14}5p^l$. We find the order to be $5s^25p^3$ in La VII followed by a successive filling of the $5p$ subshell until $5s^25p^6$ is reached in Nd VII and successive filling of the $4f$ subshell from $5s^25p^64f$ in Pm VII to $5s^25p^64f^{11}$ in Lu VII.

Carroll and O'Sullivan concluded that the $5p - 4f$ crossing occurs between the fifth and sixth ion stages (corresponding to the VI and VII spectra, respectively) from praseodymium to hafnium with some uncertainty as to its exact location. Based on our current calculations we predict a similar phenomenon but with a more gradual emptying of the $5p$ subshell, followed by emptying of the $4f$ subshell e.g. from Pr VII - Pr XI. This confirms the point made in [22] that near the location where $5p - 4f$ crossing occurs, the lowest configurations may contain both $4f$ and $5p$ electrons, the $5p$ subshell being only partially depopulated. As previously stated, this method of determining ground-state configurations is based on configuration average energies (E_{av}). In many cases E_{av} for different configurations lie very close to the ground-state configuration e.g. Nd IX: $5s^25p^4$ lies just 0.707 eV above $5s^25p^34f$. Also there is a very large spread in energy levels for some of these low lying configurations e.g. Gd VIII: $5s^25p^54f^4$ spans ≈ 33 eV. Therefore the E_{av} of one configuration could lie below the E_{av} of another configuration but above the lowest energy level of the later

configuration. In such a case the former configuration could no longer be considered as the ground-state configuration. The origin of the exact ground-state term is uncertain, and is best described as $(5s5p4f)^q$ where q is the total number of electrons shared amongst $5s$, $5p$ and $4f$ orbitals [35]. However in the absence of experimentally determined energy levels, and the presence of configuration mixing which makes state labeling somewhat ambiguous, the current approach based on E_{av} values is deemed acceptable.

III. UNRESOLVED TRANSITION ARRAYS OF LANTHANIDE IONS

In the lanthanides the strongest lines occurring in the extreme UV result from $4d - 4f$ and $4p - 4d$ transitions in ion stages with open $4d$ subshells. Since experimental information is largely lacking for these ions, it is currently not possible to estimate the necessary scaling factors used in the Cowan code for each ion stage of the different elements considered here. Therefore for consistency we decided on an *ab initio* approach and calculations were performed with the FAC code [37]. This uses a fully relativistic approach based on the Dirac equation, thus allowing its application to ions with large values of nuclear charge. The following basis set was used: $4p^6 4d^N$, $4p^6 4d^{N-1} nl$ and $4p^5 4d^{N+1}$ where $n \leq 8$, $l \leq 3$ and $1 \leq N \leq 10$. In a recent study [31] we found that for a range of 24 ions, namely, Gd^{16+} - Gd^{27+} and Tb^{17+} - Tb^{28+} , the FAC spectra were always positioned at slightly shorter wavelength than the experimental and/or the Cowan spectra. Hence a wavelength correction was subsequently applied to the FAC spectrum calculated for each ion. The largest shift necessary was ≤ 0.2 nm, which gives an estimate of the accuracy of the FAC results. For this reason we employ the FAC code in this work and all spectra presented in Figs. 2 - 4 are left unshifted due to lack of detailed experimental data for comparison.

The effect of configuration interaction for Pd-like to Rb-like ions in La to Pr is presented in Fig. 2 (non-CI on the left and CI on the right). CI leads to a narrowing of the peak for all ions considered especially at the beginning of the lanthanide series. Comparison of Mandelbaum *et al's* study [23] and the present spectra show good agreement between Rh-like, Ru-like, Sr-like and Rb-like praseodymium. The $4d - 4f$ and $4p - 4d$ subsets of the full CI UTA were extracted and are also shown in Figs. 2 - 4 in black and orange (gray) respectively (all other non $n = 4 - n = 4$ transitions appear in yellow (light gray)). The $4d - 4f$ and $4p - 4d$ UTAs are seen to overlap considerably in the early lanthanides. However

within a given element, e.g. Tb^{19+} - Tb^{28+} , both the $4d$ - $4f$ and the $4p$ - $4d$ UTAs shift to longer wavelength with the $4d$ - $4f$ shift being more prominent. This effect is observed across the lanthanide series until eventually in elements towards the end e.g. Yb and Lu, particularly in higher ion stages, these UTAs are seen to be separated considerably. This effect will be further investigated in a future work on post-lanthanide elements. However as these shifts are only minor, the net result is that the position of the peak emission (highest gA values) for a given lanthanide element is seen to remain relatively unchanged as observed for Pr in [23]. In this work a very small variation of the mean wavelength $\bar{\lambda}$ as a function of the ionization state was reported, e.g. for Pr XV - Pr XXIII, $\bar{\lambda}$ varies only from $80.7 - 83.8\text{\AA}$. This compares favorably with our current calculations where the wavelength at which maximum peak emission occurs is found to vary only from $80.24 - 83.25\text{\AA}$ for the same ions.

The above results are summarized succinctly in Fig. 5: (a) shows for each lanthanide element, the ion stage responsible for peak emission in this wavelength range. As expected with increasing Z , peak emission moves to shorter wavelength. Note this peak emission remains comparably large in all elements and as previously stated remains relatively centered for all ion stages considered. Such a centering of the peak leads us to believe that strong emission can be achieved over a wide range of plasma conditions, should any of these elements be considered as an EUV source in the future. Fig. 5 (b) shows the dependence of \sqrt{E} on nuclear charge where E is the energy of the point of maximum intensity. Good agreement is observed between the experimental results of [21] and our current calculations, and indeed can be linked to the aforementioned shift between *ab initio* and experimental spectra. It should be noted that the shift decreases with increasing ion stage, a fact that can be traced to the behaviour of the $4f$ wavefunction and its gradual contraction. In lower ion stages, the mean radius of the $4f$ is calculated to be too low, leading to the overestimate of the Slater Condon parameters, in particular the $G^1(4d, 4f)$ integral. This is corrected for by scaling in the Cowan code. As intended by Cowan, the largest adjustment to the scaling factors is required for low ion stages and the *ab initio* values are approached at high ionization stages.

IV. CONCLUSION

Theoretical ground-state configurations of lanthanide ions calculated with the Cowan suite of codes were presented and discussed in relation to previous experimental and theoretical results. Discrepancies can be attributed to interactions between $5s$, $5p$ and $4f$ orbitals resulting in ambiguities in the assignment of ground configurations. These are best described as $(5s5p4f)^q$ where q is the total number of electrons. One hundred and eighty theoretical $4d - 4f$ and $4p - 4d$ UTA spectra for Pd-like to Rb-like ions were calculated using the FAC relativistic code. The effects of configuration interaction were investigated and results compare favorably with experiments where, for increasing nuclear charge, strong emission peaks are observed to move towards shorter wavelength. The intensity of the maximum emission peak remains comparable for all lanthanide ions and centered for ions within a given element. For these reasons it is proposed that these strong emitters could be used as EUV, XUV or soft X-ray sources in the future. Already, for example, the availability of mirrors with a peak reflectivity of $\approx 40\%$ at 6.7 nm has led to proposals to use gadolinium and terbium emission as potential sources since their peak emission occurs at this wavelength. The proposed application is for lithography beyond 13.5 nm. As more mirrors become available, the other UTA identified here may find applications in this and other fields.

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TABLE I. Configurations of the type, $5s^M 5p^K 4f^N$, included in the calculation of configuration average energies E_{av} to determine the ground-state configuration.

Sequence	M+K+N	Sequence	M+K+N
Ag-like	1	Ce-like	12
Cd-like	2	Pr-like	13
In-like	3	Nd-like	14
Sn-like	4	Pm-like	15
Sb-like	5	Sm-like	16
Te-like	6	Eu-like	17
I-like	7	Gd-like	18
Xe-like	8	Tb-like	19
Cs-like	9	Dy-like	20
La-like	11	Ho-like	21

TABLE II. Ground configurations of ions in stages V - XVII for elements Lanthanum through hafnium. Discrepancies between the current table and Table I of [22] are highlighted in bold.

	V	VI	VII	VIII	IX	X	XI	XII	XIII	XIV	XV	XVI	XVII
La	$5s^2 5p^5$	$5s^2 5p^4$	$5s^2 5p^3$	$5s^2 5p^2$	$5s^2 5p$	$5s^2$	$5s$	$4d^{10}$	$4d^9$	$4d^8$	$4d^7$	$4d^6$	$4d^5$
Ce	$5s^2 5p^6$	$5s^2 5p^5$	$5s^2 5p^4$	$5s^2 5p^3$	$5s^2 5p^2$	$5s^2 5p$	$5s^2$	$5s$	$4d^{10}$	$4d^9$	$4d^8$	$4d^7$	$4d^6$
Pr	$5p^6 4f$	$5s^2 5p^6$	$5s^2 5p^5$	$5s^2 5p^4$	$5s^2 5p^3$	$5s^2 5p^2$	$5s^2 4f$	$5s^2$	$5s$	$4d^{10}$	$4d^9$	$4d^8$	$4d^7$
Nd	$5p^6 4f^2$	$5p^6 4f$	$5s^2 5p^6$	$5s^2 5p^5$	$5p^3 4f$	$5p^2 4f$	$5s^2 4f^2$	$5s^2 4f$	$5s^2$	$5s$	$4d^{10}$	$4d^9$	$4d^8$
Pm	$5p^6 4f^3$	$5p^6 4f^2$	$5p^6 4f$	$5p^5 4f$	$5p^3 4f^2$	$5p^2 4f^2$	$5s^2 4f^3$	$5s^2 4f^2$	$5s^2 4f$	$5s^2$	$4f$	$4d^{10}$	$4d^9$
Sm	$5p^6 4f^4$	$5p^6 4f^3$	$5p^6 4f^2$	$5p^5 4f^2$	$5p^3 4f^3$	$5p^2 4f^3$	$5s^2 4f^4$	$5s^2 4f^3$	$5s^2 4f^2$	$5s^2 4f$	$5s 4f$	$4f$	$4d^{10}$
Eu	$5p^6 4f^5$	$5p^6 4f^4$	$5p^6 4f^3$	$5p^5 4f^3$	$5p^3 4f^4$	$5p^2 4f^4$	$5s^2 4f^5$	$5s^2 4f^4$	$5s^2 4f^3$	$5s^2 4f^2$	$5s 4f^2$	$4f^2$	$4f$
Gd	$5p^6 4f^6$	$5p^6 4f^5$	$5p^6 4f^4$	$5p^5 4f^4$	$5p^4 4f^4$	$5p^2 4f^5$	$5s^2 4f^6$	$5s^2 4f^5$	$5s^2 4f^4$	$5s^2 4f^3$	$5s 4f^3$	$4f^3$	$4f^2$
Tb	$5p^6 4f^7$	$5p^6 4f^6$	$5p^6 4f^5$	$5p^5 4f^5$	$5p^4 4f^5$	$5p^2 4f^6$	$5s^2 4f^7$	$5s^2 4f^6$	$5s^2 4f^5$	$5s^2 4f^4$	$5s 4f^4$	$4f^4$	$4f^3$
Dy	$5p^6 4f^8$	$5p^6 4f^7$	$5p^6 4f^6$	$5p^5 4f^6$	$5p^4 4f^6$	$5p^2 4f^7$	$5p 4f^7$	$5s^2 4f^7$	$5s^2 4f^6$	$5s^2 4f^5$	$5s^2 4f^4$	$4f^5$	$4f^4$
Ho	$5p^6 4f^9$	$5p^6 4f^8$	$5p^6 4f^7$	$5p^5 4f^7$	$5p^4 4f^7$	$5p^2 4f^8$	$5p 4f^8$	$5s^2 4f^8$	$5s^2 4f^7$	$5s^2 4f^6$	$5s^2 4f^5$	$4f^6$	$4f^5$
Er	$5p^6 4f^{10}$	$5p^6 4f^9$	$5p^6 4f^8$	$5p^5 4f^8$	$5p^4 4f^8$	$5p^2 4f^9$	$5p 4f^9$	$5s^2 4f^9$	$5s^2 4f^8$	$5s^2 4f^7$	$5s^2 4f^6$	$5s 4f^6$	$4f^6$
Tm	$5p^6 4f^{11}$	$5p^6 4f^{10}$	$5p^6 4f^9$	$5p^6 4f^8$	$5p^4 4f^9$	$5p^2 4f^{10}$	$5p 4f^{10}$	$5s^2 4f^{10}$	$5s^2 4f^9$	$5s^2 4f^8$	$5s^2 4f^7$	$5s 4f^7$	$4f^7$
Yb	$5p^6 4f^{12}$	$5p^6 4f^{11}$	$5p^6 4f^{10}$	$5p^6 4f^9$	$5p^4 4f^{10}$	$5p^3 4f^{10}$	$5p 4f^{11}$	$5s^2 4f^{11}$	$5s^2 4f^{10}$	$5s^2 4f^9$	$5s^2 4f^8$	$5s 4f^8$	$4f^8$
Lu	$5p^6 4f^{13}$	$5p^6 4f^{12}$	$5p^6 4f^{11}$	$5p^6 4f^{10}$	$5p^4 4f^{11}$	$5p^3 4f^{11}$	$5p 4f^{12}$	$5s^2 4f^{12}$	$5s^2 4f^{11}$	$5s^2 4f^{10}$	$5s^2 4f^9$	$5s 4f^9$	$4f^9$

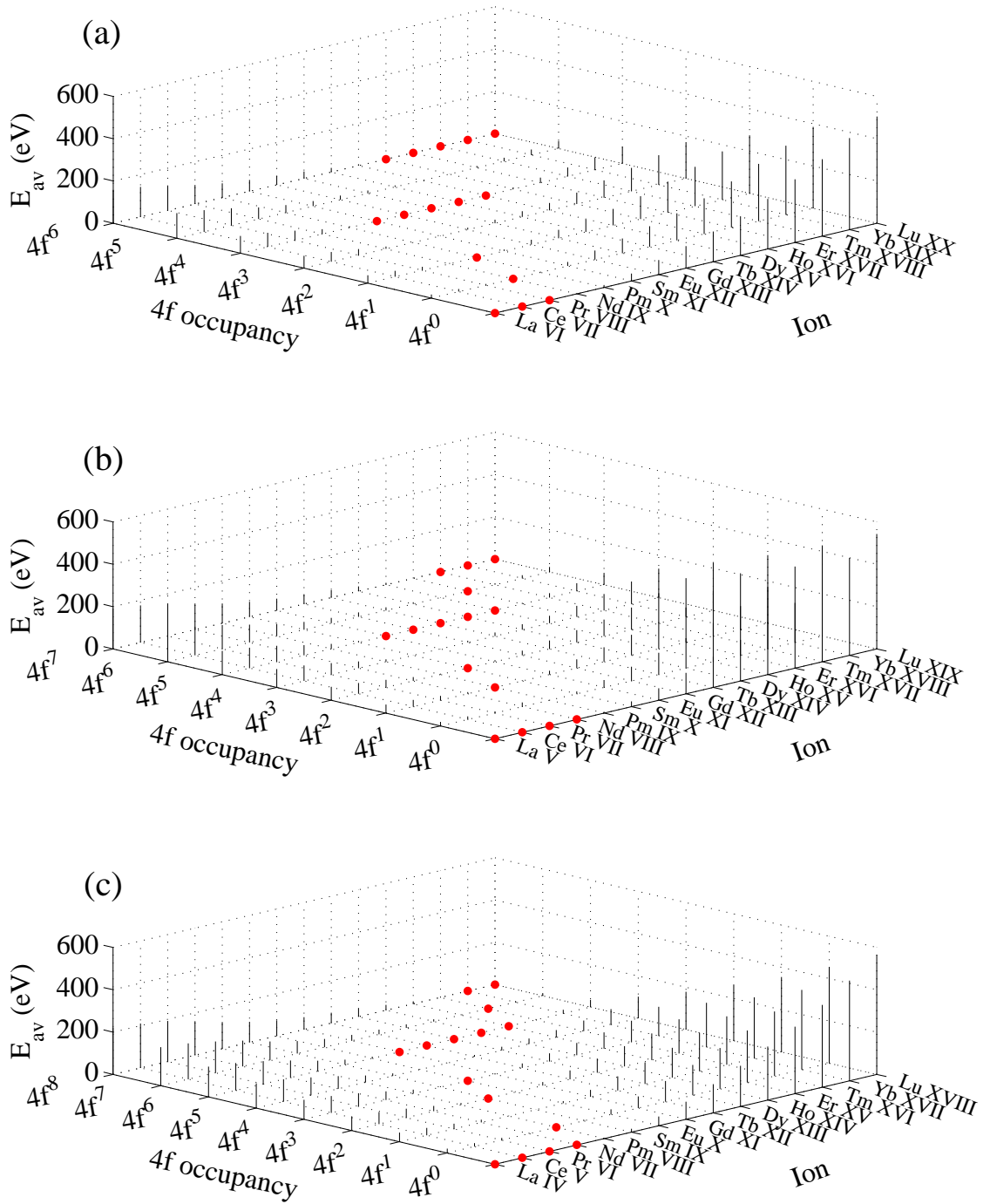


FIG. 1. (Color online) Configuration average energies E_{av} of the Te-like to Xe-like ions: (a) Te-like, (b) I-like and (c) Xe-like ions (red (dark gray) dot denotes ground configuration).

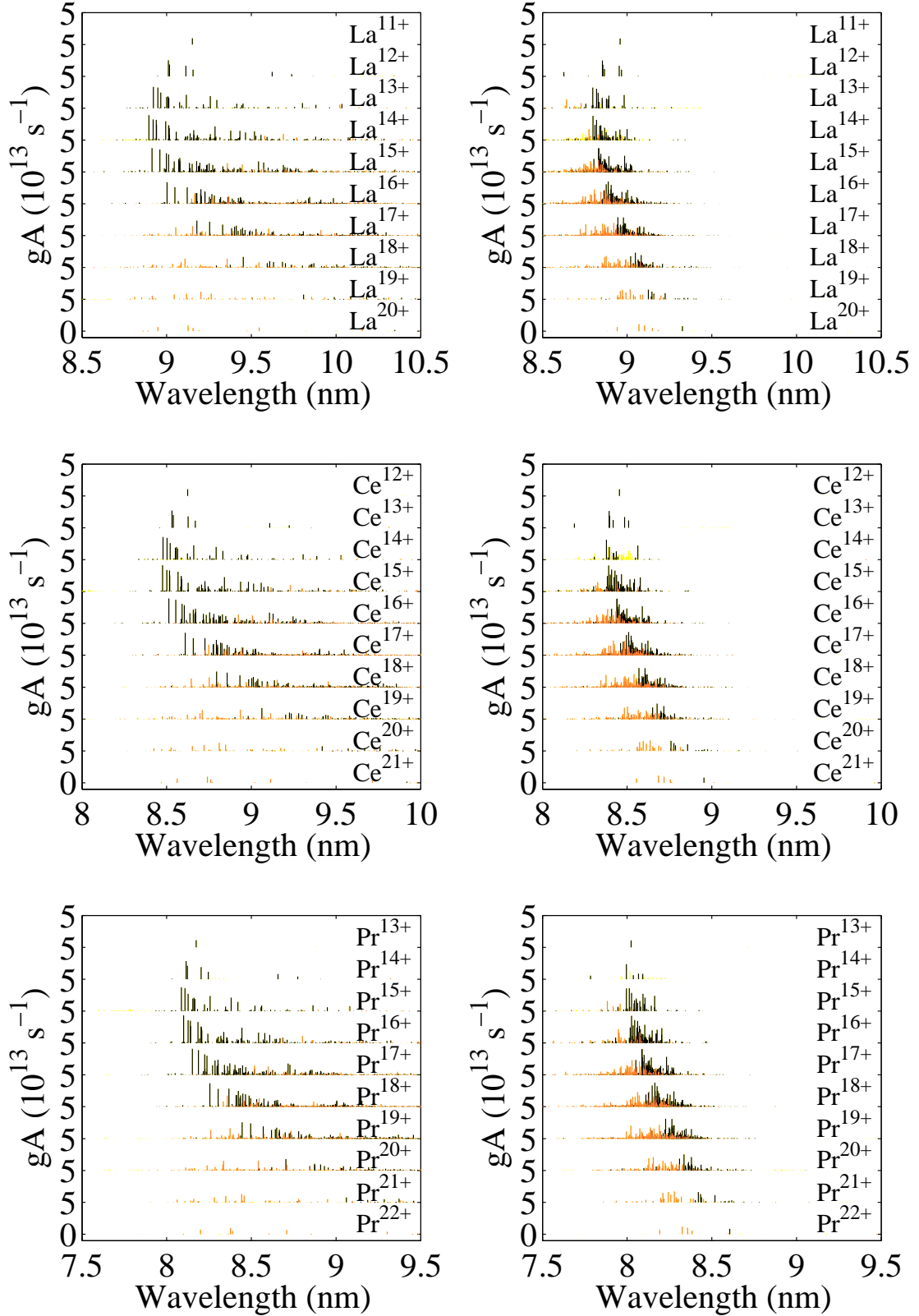


FIG. 2. (Color online) Pd-like through Rb-like spectra of lanthanum, cerium and praseodymium computed with the FAC code, excluding CI (left) and including CI (right). Black denotes $4d - 4f$ transitions, orange (gray) denotes $4p - 4d$ transitions and yellow (light gray) denotes all transitions.

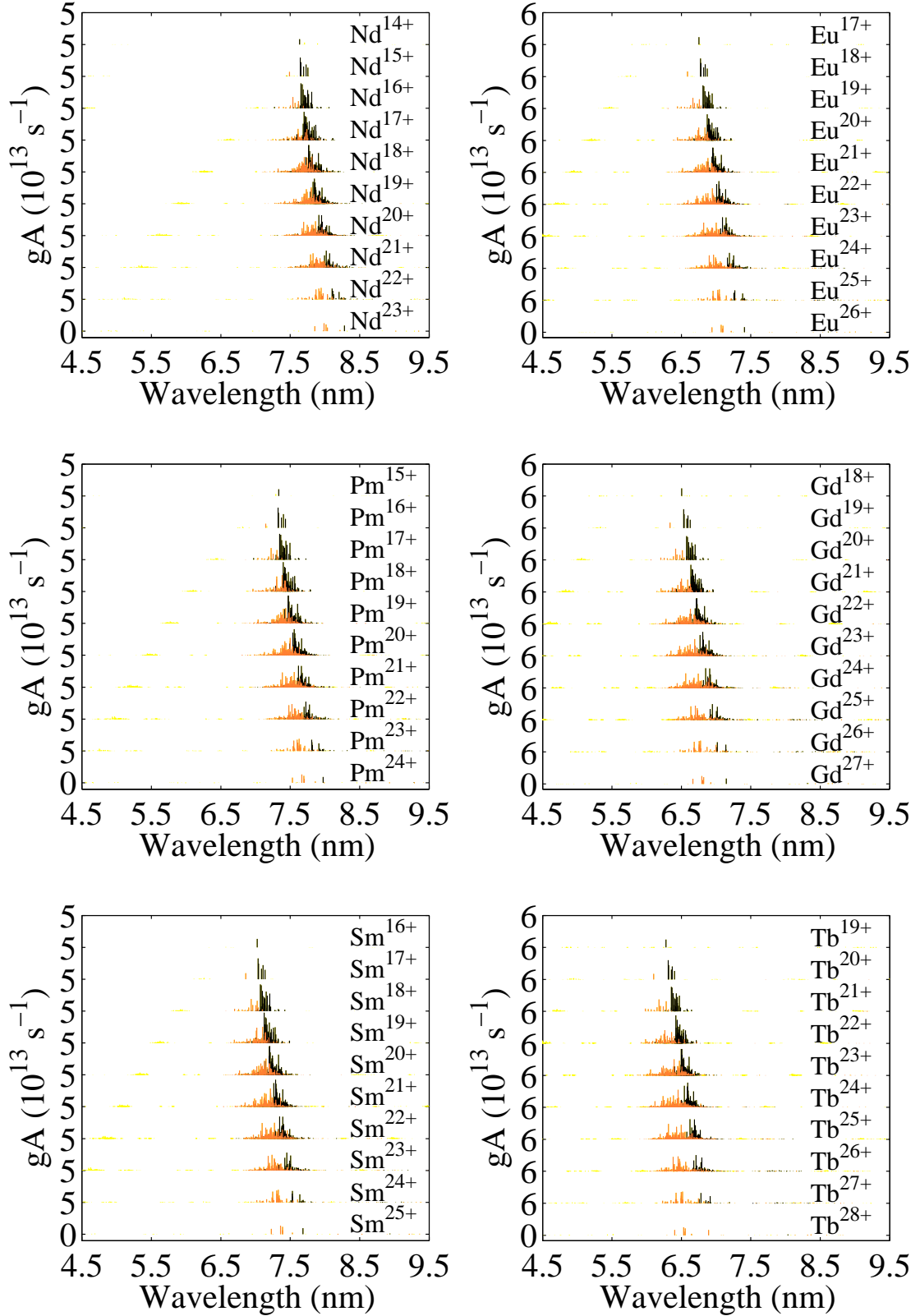


FIG. 3. (Color online) Pd-like through Rb-like spectra of neodymium through terbium computed with the FAC code including CI. Black denotes $4d - 4f$ transitions, orange (gray) denotes $4p - 4d$ transitions and yellow (light gray) denotes all transitions.

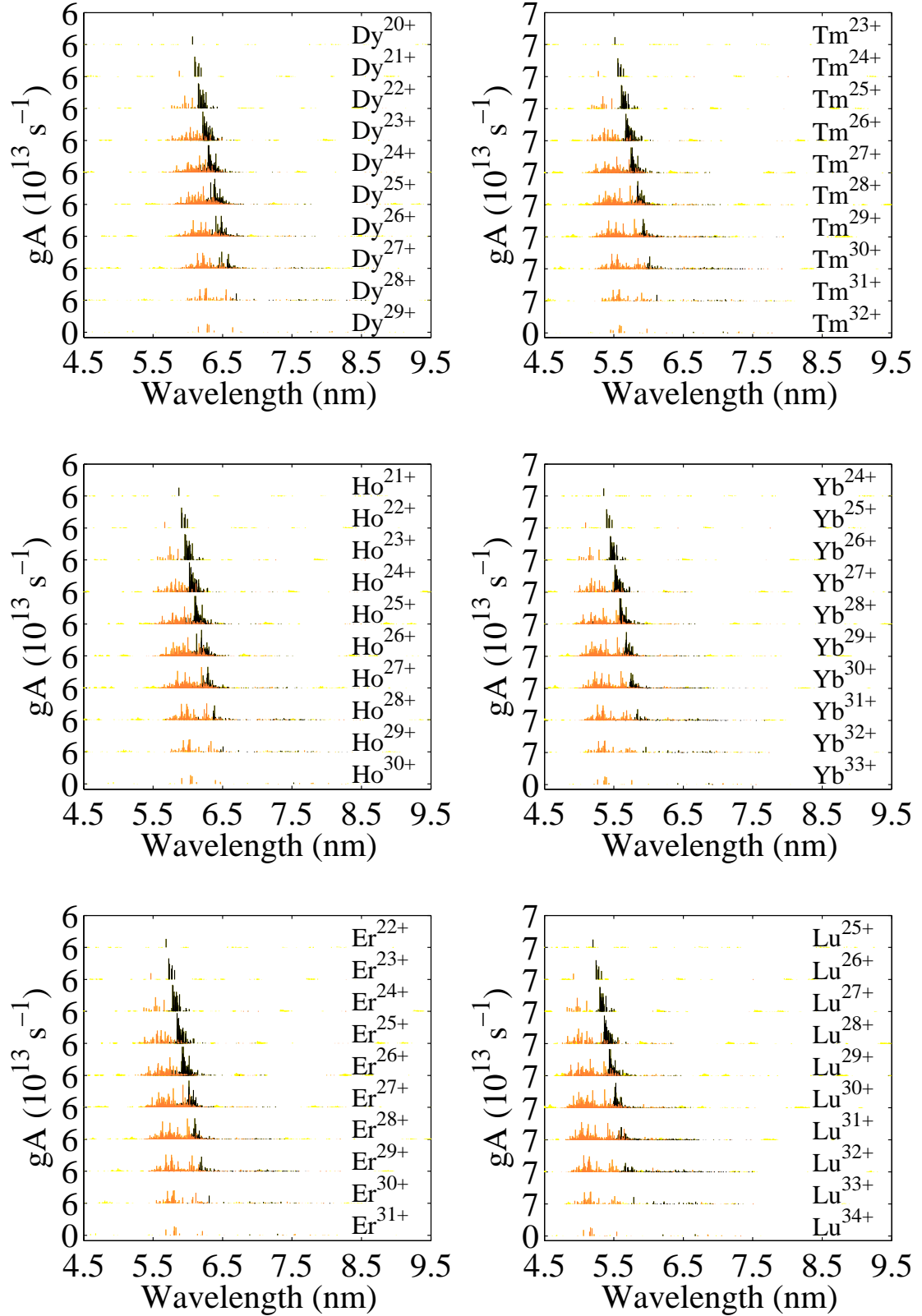


FIG. 4. (Color online) Pd-like through Rb-like spectra of dysprosium through lutetium computed with the FAC code including CI. Black denotes $4d - 4f$ transitions, orange (gray) denotes $4p - 4d$ transitions and yellow (light gray) denotes all transitions.

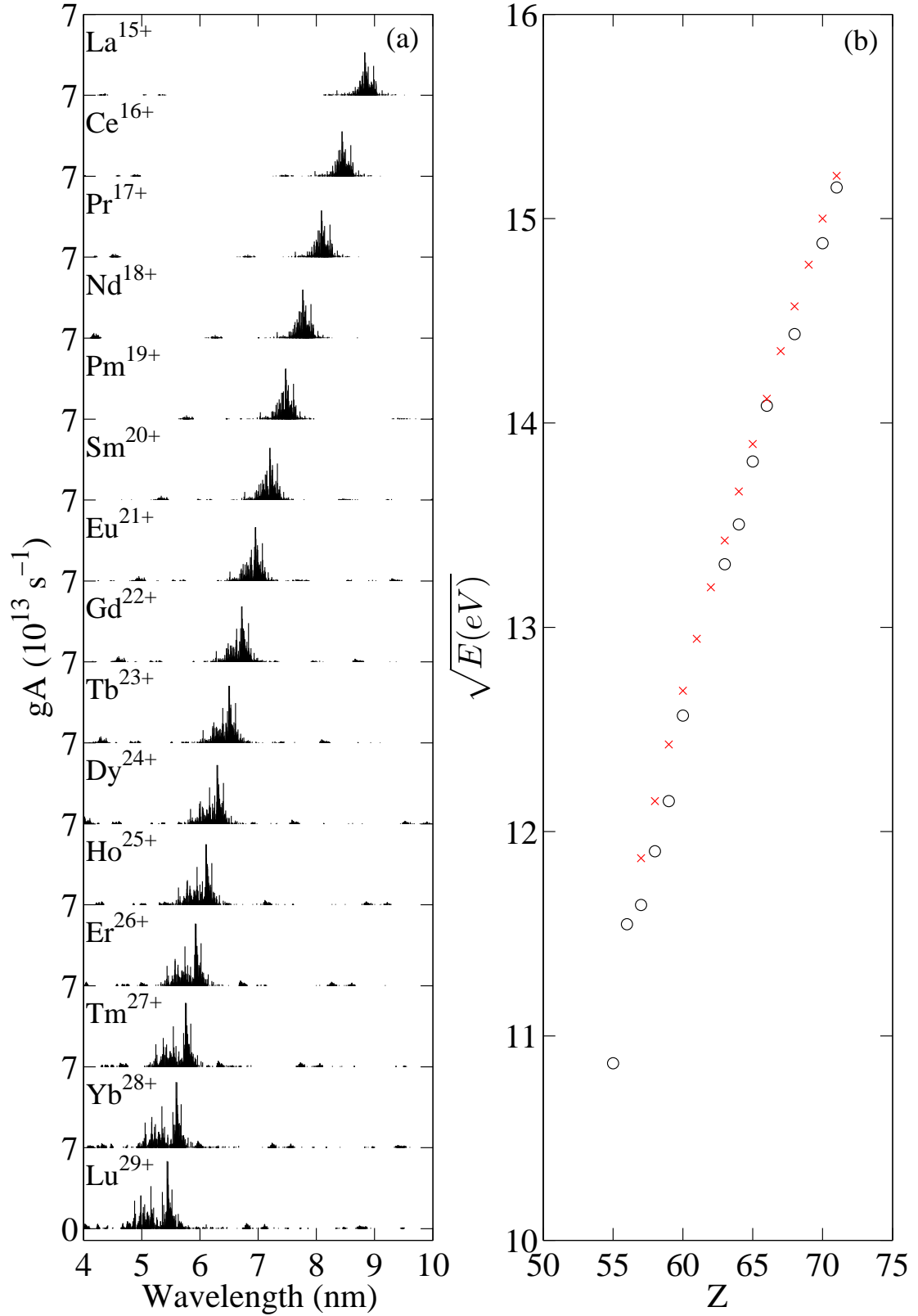


FIG. 5. (Color online) (a) Maximum peak emission from $4d - 4f$ and $4p - 4d$ UTAs (including CI) in the lanthanide series. (b) Dependence of UTA transition energies on atomic number Z . Black open circles, $4d - 4f$ [21], red (dark gray) crosses, current work.