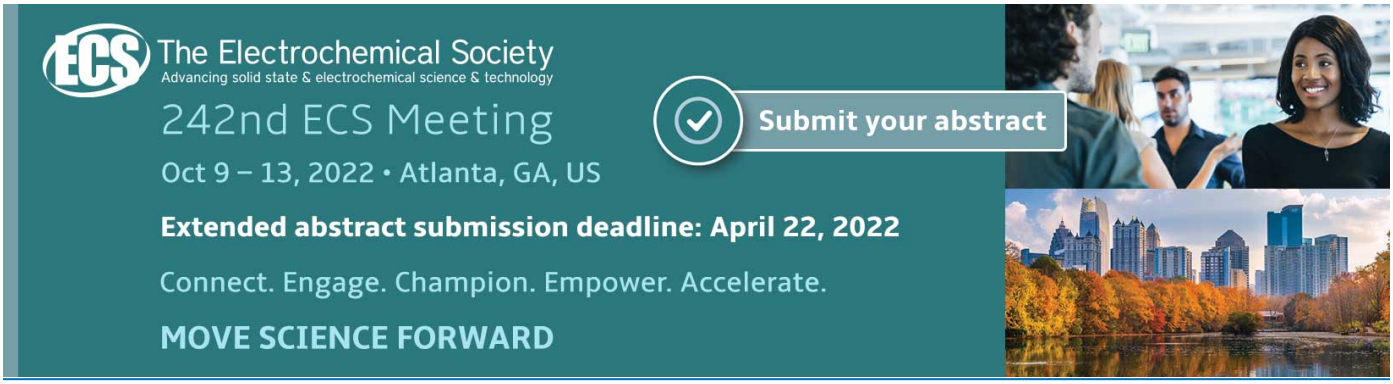
Radiative and Auger cascades in Fe^{3+}



Radiative and Auger cascades in Fe^{3+}

V Jonauskas[1]*, P Drabužinskis[1], S Kučas[1] and J Koncevičiūtė[1]

[1]Vilnius University, Institute of Theoretical Physics and Astronomy, Saulėtekio av. 3, Vilnius, LT-10257, Lithuania

Synopsis Radiative and Auger cascades following creation of the $2s$ or $2p$ shell vacancy in the Fe^{2+} ion are studied by performing calculations for energy levels and subconfigurations. Radiative and Auger spectra and charge state distribution determined by cascade are investigated. Branching ratios of the cascade are analyzed and main decay mechanisms are identified for all levels of the studied configurations.

Electromagnetic emission from accretion disk of active galactic nucleus is the main source that determines higher ionization stages in the surrounding matter. Inner-shell vacancy created by photon leads to cascade of radiative and Auger transitions. Spectral lines of the Fe^{2+} and Fe^{3+} ions were observed in active galactic nuclei [1, 2]. Therefore, the higher ionization stages of iron can be also produced in such objects.

The aim of the current work is to study radiative and Auger cascade following the creation of L shell vacancy in Fe^{2+}. Energy levels, electric dipole and Auger transitions are calculated using Flexible Atomic Code (FAC) [3] which implements the Dirac-Fock-Slater approach. Atomic data are studied using single-configuration approximation. Previous calculations for cascade were performed by considering transitions among configurations [4].

The main decay channels from the lowest level of the $2s\,3d^6$ configuration following the $2s$ shell vacancy creation for Fe^{2+} are shown in Fig. 1. Population transfer from Fe^{4+} $2p^53d^5$ is not presented in this figure. The strongest branch corresponds to $Fe^{3+}\,2s\,3d^6 \rightarrow Fe^{4+}2p^53d^5 \rightarrow Fe^{5+}3p^43d^5$ (26%) sequence of transitions. Auger decay of $Fe^{5+}3p^43d^5$ transfers only 0.5% of population to $Fe^{6+}\,3p^53d^3$. The study demonstrates that the highest ion yield corresponds to Fe^{5+} ($\sim 80\%$). The highest ionization stage produced by cascade reaches Fe^{7+}, however, with very low population ($< 1\%$). It has to be noted that ion yield depends on the initial level of the $2s\,3d^6$ configuration. This configuration has 63 energy levels. Variation of population for Fe^{5+} is less than 10% for the different levels of the initial configuration. The ground $3d^3$ configuration of Fe^{5+} is mainly populated in the cascade. However, small part of population ($< 5\%$) appears in the long lived levels of the excited $3p^53d^4$ configuration.

Decay of the Fe^{3+} $2p^53d^6$ vacancy reaches Fe^{6+}. There are 180 energy levels of the $2p^53d^6$ configuration. Population of ions depends on the initial level the cascade starts. Variation of the population for the Fe^{6+} ion from 0.2% to 8.1% is obtained for the different initial levels. The main decay branches of cascade from the lowest level of Fe^{3+} $2p^53d^6$ are $Fe^{3+}\,2p^5\,3d^6 \rightarrow Fe^{4+}\,3p^43d^6 \rightarrow Fe^{5+}\,3p^53d^4$ (23%) and $Fe^{3+}\,2p^5\,3d^6 \rightarrow Fe^{4+}\,3s\,3p^53d^6 \rightarrow Fe^{5+}\,3p^53d^4$ (9%).

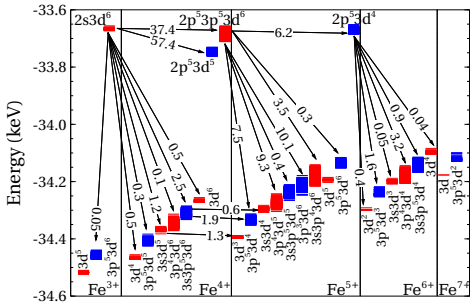


Figure 1. Radiative and Auger cascade corresponding to decay of the Fe^{3+} $2s\,3d^6$ configuration. Blue (dark) represents even parity configurations; red (light) represents odd parity configurations.

References

[1] Laor A *et al* 1997 *Astrophys J* **489** 656
[2] Vestergaard M *et al* 2001 *Astrophys J Suppl Ser* **134** 1
[3] Gu M F 2008 *Can J Phys* **86** 675
[4] Kaastra J S *et al* 1993 *Astron Astrophys Suppl Ser* **97** 443

*E-mail: valdas.jonauskas@tfai.vu.lt