Accurate Calculations of Auger Cascade for Medical and Physical Applications

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Auger electrons and characteristic X-rays, collectively named as atomic radiation, are emitted following atomic ionization. Radioisotopes that emit Auger electrons have been of particular interest as therapeutic agents. This is primarily due to its short range in tissue, controlled linear paths and high linear energy transfer of these particles. Their biological effect is very localised thus making nuclear targeted Auger-electron emitters ideal for precise targeting of cancer cells. Accurate knowledge of Auger yields is needed both to evaluate the dose to healthy cells when radioisotopes are administered for diagnostics, and to design radioisotope use in the targeted cancer therapy.

A pilot computational model of Auger cascade, which is based on a Monte Carlo method, using up-to-date nuclear input data and atomic transition probabilities from evaluated atomic data library (EADL) [1], has been developed. Details of the model and results for ^{99m}Tc, ^{111}In, ^{123}I, ^{125}I, ^{131}Cs and ^{201}Tl, have been published [2, 3]. *Ab initio* calculations of atomic transition energies are performed at every propagation step of the Auger cascade using relativistic Dirac-Fock (DF) method. The Auger-energy spectra and the charge distributions of the residual atoms following nuclear decay have been calculated and compared with available experimental data. Reasonably good agreements with experimental results have been achieved. However, the pilot model is restricted by the lack of QED corrections for binding energies in standard relativistic DF method [4]. Besides, the atomic data from EADL [1], which is calculated for single initial vacancy, is not suitable for the Auger cascade in a multiply ionised atom.

Multiconfigurational Dirac-Fock (MCDF) method has been found a versatile tool for calculating a variety of atomic properties. Computer codes GRASP2K [5] and RATIP [6] based on MCDF method are adapted to overcome the current limitations of the pilot model. One of the advantages that GRASP2K and RATIP offer is the intensive treatment of QED effects. Comparison of MCDF calculations with recent experimental data for several radioisotopes will be presented. The calculated results of K Auger transitions are generally in much greater agreements with available experimental data.

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