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Multiple electron processes from H_2O by He^{2+} and Li^{3+} impact

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Synopsis We employ the Continuum Distorted Wave-Eikonal Initial State approximation for He^{2+} and Li^{3+} ions impacting on water vapor targets to study multiple electron removal processes at the intermediate to high projectile energy range. Transition probabilities and absolute cross sections for pure ionization, capture and transfer-ionization channels were calculated. Results are compared with previous calculations and recent experimental data.

Investigation of single and multiple-electron removal processes occurring between fully stripped ions and H_2O molecules is of fundamental interest in many areas such as nuclear fusion [1], plasma physics [2] and others. In particular, it is of fundamental importance in radiotherapy [3] enabling the understanding of the basic governing mechanisms involved. A large variety of final projectile and target charge states may be produced during these processes. Consequently, calculations of cross sections of pure ionization, capture and transfer-ionization reactions are essential to determine the main features of multiple electron processes.

He^{2+} and Li^{3+} beams are chosen in this work. The three-body Continuum Distorted Wave-Eikonal Initial State approximation (3B-CDW-EIS) [4] is used to calculate transition probabilities (capture and ionization) as a function of the impact parameter and absolute cross sections for the considered collisions. The initial wave-functions of the active electrons bound to a particular water molecular orbital are described employing the complete neglect of the differential overlap (CNDO) approximation [5]. A trinomial distribution analysis has been employed to compute exclusive probabilities using the independent electron (IEL) model, where electron correlation is neglected [6]. A unitarization procedure is employed to avoid overestimations of 3B-CDW-EIS impact parameter probabilities.

From the comparison with the available theoretical and recent experimental results, we conclude that inclusive probabilities are required for a reliable description of the processes of interest for single-electron removal processes (see Figure 1) and exclusive probability analysis for multiple-electron ones.

The developed method for calculation of one-electron ionization and capture probabilities allows to study multiple electron processes for complex targets in particular such as macromolecules of DNA and RNA to model scenarios for the radiobiological consequences of the impact of charged energetic particles on those macromolecules.

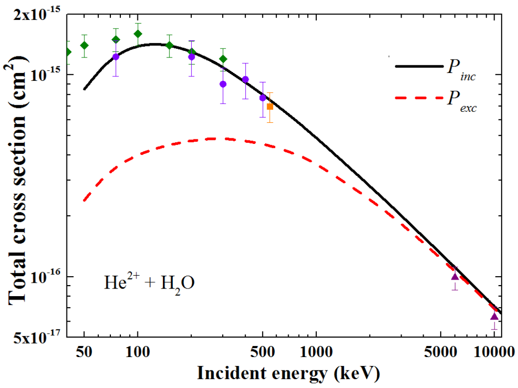

Figure 1. Total single ionization cross sections as a function of the incident energy for He^{2+} impacting on H_2O.

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References

[1] S. Yu Simon *et al.* 2007 *Nucl. Fusion* **47** 721-727

[2] I. Murakami, J. Yan, H. Sato, M. Kimura, R.K. Janev, T. Kato 2008 *At. Data Nucl. Data Tables* **94** 161-222

[3] D. Schardt, T. Elsässer and D. Schulz-Ertner 2010 *Rev. Mod. Phys.* **82** 383-425

[4] P.D. Fainstein, V.H. Ponce and R.D. Rivarola 1991 *Phys. B: At. Mol. Opt. Phys.* **24** 3091-3119

[5] J. Pople, D. Santry and G. Segal 1965 *J. Chem. Phys.* **43** S136-S151

[6] J. Bradley, R. J. S Lee, M. McCartney and D. S. F. Crothers 2004 *J. Phys. B: At. Mol. Opt. Phys.* **37** 3723-373