66th OSU INTERNATIONAL SYMPOSIUM ON MOLECULAR SPECTROSCOPY

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FB. THEORY

FRIDAY, JUNE 24, 2011 – 8:30 am

Room: 170 MATH ANNEX

Chair: JOHN HERBERT, The Ohio State University, Columbus, Ohio

FB01 **15 min 8:30**

AUGER ELECTRONS VIA K_α X-RAY LINES OF PLATINUM COMPOUNDS FOR NANOTECHNOLOGICAL APPLICATIONS

SULTANA N. NAHAR, *Dept of Astronomy, The Ohio State University, Columbus, OH 43210*; SARA LIM, *Biophysics Program, The Ohio State University, Columbus, OH 43210*; A.K. PRADHAN, *Dept of Astronomy, and Chemical Physics Program, The Ohio State University, Columbus, OH 43210*; R.M. PITZER, *Dept of Chemistry, The Ohio State University, Columbus, OH 43210.*

We will report study on the K_α X-ray lines of platinum. Pt compounds, such as cisplatin, are common in biomedical applications. The active element Pt can emit or absorb hard X-rays. We have obtained the photoionization cross sections from the oscillator strengths of 1s-2p (K_α) transitions in Pt ions. We find that these transitions appear as resonances in photoionization in the hard X-ray energy range of 64 - 71 keV (0.18 - 0.17 Å below the K-shell ionization and with a strength orders of magnitude higher compared to that at the K-shell ionization. This is the focus of our study for possible initiation of an emission cascade of Auger electrons at the resonant energy. We will present the oscillator strengths and attenuation coefficients per unit mass for all the K_α transitions in the event platinum cascades through various, namely from fluorine-like to hydrogen like, ionic states. The study is motivated by uur proposed method, *Resonant Theranostics*[b,c] (RT) for biomedical appliations, which aims to find narrow band X-ray energy that corresponds to *resonant* photo-absorption and leads to emission of Auger electrons. As the next step of the RT method we will also report on experimental results on producing monochromatic X-rays, targeted to the resonant energy, from the wide band Bremstruhlung radiation of a conventional X-ray source.
a b c

[a]Partially support: DOE, Computational Facility: Ohio Supercomputer Center, Columbus, Ohio.

[b]"Resonant X-Ray Enhancement of the Auger Effect in High-Z atoms, molecules, and Nanoparticles: Biomedical Applications", A.K. Pradhan, S.N. Nahar, M. Montenegro, Yan Yu, H.L. Zhang, C. Sur, M. Mrozik, R.M. Pitzer, J. of Phys. Chem. A, 113 (2009), 12356.

[c]"Monte Carlo Simulations and Atomic Calculations for Auger Processes in Biomedical Nanotheranostics", M. Montenegro, S. N. Nahar, A. K. Pradhan, Ke Huang, Yan Yu, J. of Phys. Chem. A, 113 (2009), 12364.

FB02 **15 min 8:47**

A QUANTUM CHEMICAL EXPLORATION OF THE SF_nO SERIES ($n = 1 - 5$): AN ATOM-BY-ATOM APPROACH

TYLER Y. TAKESHITA, D. E. WOON, and T. H. DUNNING, JR., *Department of Chemistry, University of Illinois at Urbana-Champaign, Urbana, IL 61801.*

The recoupled pair bonding model and high level ab initio calculations (MRCI, RCCSD(T)) with correlation consistent basis sets were used to examine the optimized structures, transition states, bonding and bond energies of the SF_nO series ($n = 1-5$). Oxygen is capable of participating in covalent, recoupled pair, and dative bonding and, unlike monovalent ligands, forms both σ and π bonds. This study explores the effect of oxygen in order to anticipate its impact on trends in bond energy and other properties similar to those observed in previous SF_n ($n = 1 - 6$) recoupled pair bonding studies. Of particular interest are those states that are either formed as a result of decoupling a pair of electrons or by further addition to a molecule that has already undergone the decoupling process.