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FE07 **15 min 10:32**

ATOMIC SPECTROSCOPY: ASTRONOMY TO BIO-MEDICAL SCIENCE

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Spectroscopy is the main step to understanding the details of the universe. Under the Iron Project (IP), an international collaboration of countries US, UK, France, Germany, Belgium, and Venezuela, we have been carrying out systematic study of radiative and collisional atomic processes, including atomic spectroscopy, of iron-peak elements abundant in astronomical objects. We have developed the method, relativistic Breit-Pauli R-matrix in close coupling approximation, to calculate large number of fine structure energy levels and transitions among them and procedure to identify the levels spectroscopically by employing quantum defect analysis, interacting channel contributions, LS- and JJ-coupling algebra. I will discuss these with astrophysical applications. One important aspect, highly relevant to Pitzer symposium, will be X-ray spectroscopy of heavy elements and its application especially to biomedical science under our interdisciplinary program that Russ Pitzer has been involved for about 4 years. Heavy elements produce hard X-rays with with large attenuation coefficients and can be implemented in cancer theranostics. [a] [b]

[a] Acknowledgement: Partially supported by a Large Interdisciplinary Grant award, the Ohio State University. The computational work was carried out on the Cray X1 and Itanium 4 cluster at the Ohio Supercomputer Center, Columbus Ohio.

[b] "Resonant X-ray Irradiation of High-Z Nanoparticles For Cancer Theranostics", Anil Pradhan, Sultana Nahar, Max Montenegro, Chiranjib Sur, Mike Mrozik, Russ Pitzer, Yan Yu, Eric Silver, *Ohio Nanotechnology Summit 2007*, April 24-25, Akron, Ohio, Poster Sessions and Abstracts, NB-3, p.37

FE08 **10 min 10:49**

ELECTRONIC STRUCTURE AND SPECTROSCOPY OF THE MgO_2^+ CATION

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Highly correlated *ab initio* methods are used to investigate the lowest MgO_2^+ electronic states. Our computations confirm the existence of the strongly bent (MgO_2^+ X^2 A_2) form and the weakly bound *l*-MgOO^+ (X^4 Σ^-) charge quadrupole complex [a].

For both isomers, the three-dimensional potential energy surfaces ($3D - PESs$) of their electronic ground states are mapped in internal coordinates not far from their respective equilibrium geometries. Then a set of spectroscopic parameters are derived using second order perturbation theory. The rovibrational spectra are also deduced variationally. One-dimensional cuts of the $3D - PESs$ of the lowest doublet and quartet electronic states of MgO_2^+ along the R_{MgO} and R_{OO} stretching and bending coordinates, are calculated, covering both the molecular ans the asymptotic regions. These curves are used later in order to discuss the metastability of these electronic states and to propose mechanisms for the $Mg^+ + O_2$ atmospheric ion-molecule reaction. [b].

[a] M. Sodupe and C.W. Bauschlicher, Jr., *Chem.Phys.Lett.*, **203**, 215 (1993)

[b] O. Yazidi, A. Ben Houria, Z. Ben Lakhdar, M.L. Senent and M. Hochlaf (submitted, 2008)