Spin-Orbit Coupling of the 5f Electrons In Actinide Oxides

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Presented by…

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Abstract: The coupling of the spin and orbital angular momentum of the electrons in the open shells of transition metal, rare-earth, and actinide cations is important, especially for the magnetic properties of oxides and other ionic compounds. When relativistic spin-orbit splitting is small, as for the 3d transition metal oxides, a maximum spin alignment of the open shell electrons explains the properties of high spin ionic crystals. For actinide cations, where the spin-orbit splitting of the 5f shell into 5f5/2 and 5f7/2 is much larger than for the 3d shell, there is a competition between aligning the spins of the 5f electrons and filling first the lower lying 5f5/2 sub-shell. This competition often leads to a significantly reduced spin alignment and, hence, a smaller magnetic moment. Novel concepts are used to explain the dependence of the spin alignment on the 5f shell occupation. The consequences of this spin-alignment for the magnetic moment are examined for metal cations and for embedded clusters modeling actinide oxides.

Bio: Bagus' theoretical research has focused on topics core level ionization and excitation, especially as it is relevant for X-ray photoemission spectroscopy, XPS, and X-ray Adsorption Near Edge Spectroscopy, XANES.; and the chemistry of surfaces with particular emphasis on the bonding between adsorbates and surfaces. Essentially all of his research has involved using computations to determine the electronic structure of matter. He has made major contributions to the development of methods and programs to compute this electronic structure and to analyze the computed wavefunctions.

More info:

http://cascam.unt.edu/people/psbagus.htm

Tuesday
December 18

EMSL Auditorium

10:30 am