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C076 **The Interpretation of Experimental Spectroscopic Data in Coordination Chemistry Using High Performance Computing**

Christian Knoll, Danny Müller, Peter Weinberger

Vibrational and optical spectroscopy are well known as very useful tool for the characterization of inorganic coordination compounds. With the program suite Gaussian09 rev.C using VSC-1 and VSC-3 theoretical molecular spectroscopy is carried out and compared to experimental data in the field of small molecule organic chemistry and coordination chemistry. Within our contribution some of these applications of high performance computing in inorganic coordination chemistry are presented.

C092-pdp **Investigating the Excited State Photophysical Properties of Re(I) Complexes of Hexaazatrinaphthylnene with Alkyl and Thioether Substituents Using Time Resolved Vibrational Spectroscopic Techniques**

Raphael Horvath, Holly van der Salm, Jack Turner, Michael Fraser, Charlotte Clark, Samuel Lind, Xue-Zhong Sun, Keith Gordon, Michael George

Mono, bis, and tris-metallic Re(I) complexes of hexaazatrinaphthylene (HATN) with methyl substituents (HATN-Me) and thioalkyl-substituents (HATN-S) are investigated. The initially excited state is probed using resonance Raman and density functional theory calculations and the triplet excited state is probed with time resolved IR spectroscopy. The inclusion of electron-donating thioalkyl chains was found to significantly perturb the initial excitation and reduce charge-transfer in the triplet state.

Surface Science

C077 **Localization of Phase Transformation Processes in Zirconia-Based Ceramics by Topography-Based Confocal Raman Imaging**

Arne Ziebell, Johannes Ofner, Bernhard Lendl, Michael Konegger

In the past three decades, zirconia (ZrO_2)-based ceramics have been successfully established as standard structural materials for a wide variety of high-performance applications. As a model system, a tetragonal zirconia polycrystalline surface with a surface defect induced by mechanical impact was used. The objective of this work is the demonstration of the applicability of confocal Raman imaging for the differentiation between ZrO_2 modifications on a microstructural level, taking into account topographical features of a ZrO_2 surface after damage-induced failure.

C078 **In Situ Raman Spectroscopy Studies on Plasmon-Catalyzed Charge Transfer Reaction: From $TCNQF_4^-$ to $TCNQF_4^{2-}$**

Shuping Xu, Jing Wang, Weiqing Xu

We employed the Raman spectroscopy to investigate the charge transfer reaction of Ag-$TCNQF_4$ under the plasmonic catalysis.

C079 **Change in the Surface Geometry of the N-benzylamino(boronphenyl)methylphosphonic Acid Analogues Adsorbed onto Silver Nanoparticles in Alkaline Medium: SERS Studies**

Natalia Piergies, Edyta Proniewicz, John R. Lombardi

Here we present the SERS investigations of the selected group of boron analogues of aminophosphonic acids immobilized onto colloidal silver nanoparticles at the alkaline medium. These molecules are considered as potential kinase and protease inhibitors. The presented results indicate time-dependent changes in the adsorption geometry of the molecules. Briefly, within the first 15 minutes the interaction between the molecules and the colloidal silver nanoparticles, through the boronphenyl ring and the B-O bond, is observed. In time, this interaction becomes stronger.

The interpretation of experimental spectroscopic data in coordination chemistry using high performance computing

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Keywords: tetrazoles, iron(II) spin crossover, DFT, infrared spectroscopy.

Vibrational and optical spectroscopy are well known as very useful tool for the characterization of iron(II) spin crossover compounds.[1,2] With the program suite Gaussian09 rev.C using VSC-1 and VSC-3 theoretical molecular spectroscopy is carried out and compared to experimental data in the field of small molecule organic chemistry (i.e. tetrazole ligands) and the iron(II) coordination chemistry. Within our contribution some of these applications of high performance computing in inorganic coordination chemistry are presented.[2]

Fe(II) spin crossover compounds with tetrazole ligands (tz) occur in two possible spin states (LS: S=0; HS: S=2). The spin switching energy is within the range of the thermal energy, so it is possible to change the spin state by cooling or heating the compound.

Via theoretical calculations we are able to confirm experimental findings in the trend of the spin switching energy. Also spin-state dependent IR calculations are in good agreement with the variable temperature MIR/FIR spectroscopic data.

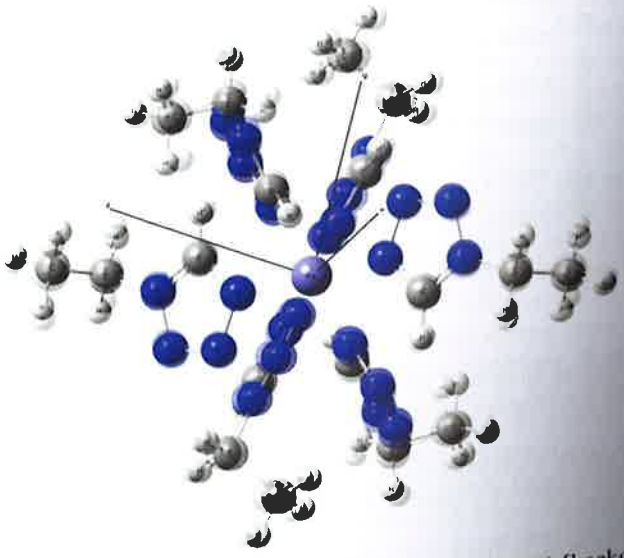

Figure 1. Overlay of $[Fe(2tz)_6]^{2+}$ (LS) [foreground] and (HS) [background]

Acknowledgements:
We gratefully acknowledge financial support from the Austrian Science Fund (FWF), project P24955-N28. Financial support of the COST project CM 1305 providing a short time scientific mission of Christian Knoll in the University of Warwick (UK) and a summer school at the university of Groningen (The Netherlands) is acknowledged. The computational results presented have been achieved using the Vienna Scientific Cluster VSC-1 and VSC-3.

[1] Weinberger P., Matthias G., (2004) *Vibrational Spectroscopy* 34(1), 175-186p.
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