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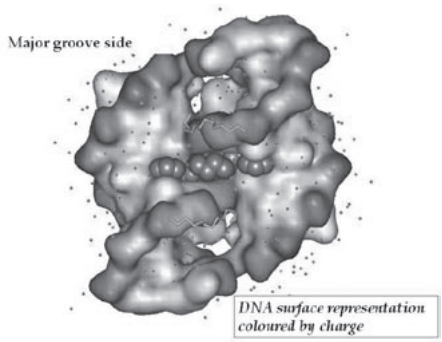
The Cardin group has recently been successful[1] in determining the modes of binding to the DNA Holliday junction of a bisintercalator. The acridine chromophores of the bisintercalator replaced two adenine bases at the junction, see Figure. The mode of binding of these so-called bisintercalators is not intercalative, but displacement of the adenosines at position 6 of the crossover strands, and their replacement with acridine groups in the AT basepair. The 4-carboxamide sidechains thread through to the minor groove side of the junction but make no specific hydrogen bond. The acridine chromophore also makes no specific interaction with the unpaired thymine. Rather, the binding is stabilised by stacking interactions, good steric fit and charge neutralisation. The Cardin group characterised the crosslinking of duplex DNA by the same compound[2]. This talk will include recent unpublished results demonstrating that recognition of the junction can take place in solution.



[1]Brogden, A.L., Hopcroft, N.H., Searcey, M., and Cardin, C.J., Angew. Chem. Internat.Edn.,2007, 46,3850-3854.
[2]Hopcroft,N.H., Brogden, A.L., Searcey, M., and Cardin, C.J., Nucleic Acids Res, 2006, 34,6663-6672.

Keywords: DNA, Holliday, intercalator

MS.94.1

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X-ray Raman scattering: A probe of soft X-ray absorption edges using hard X-rays

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Non-resonant x-ray Raman scattering has emerged as a valuable, complementary, and in some cases unique tool to study truly bulk sensitive soft x-ray absorption edges with high energy x-rays, in particular if electrons or soft x-rays are difficult to use as a probe. Nowadays, dedicated experimental endstations are accessible at third generation synchrotron radiation sources which is reflected in a strong increase of x-ray Raman scattering studies during the past decade. This development is accompanied by a considerable progress in understanding non-resonant x-ray Raman spectra theoretically. For low momentum transfers in the so-called dipole limit the measured x-ray Raman spectra can be compared with results of soft x-ray absorption studies. If the momentum transfer is increased non-dipole transitions contribute significantly to the spectra so that the unoccupied density of states can be studied symmetry selectively which has been widely used in, e.g., exciton spectroscopy. Although the main focus of such experiments was set on the study of the very near edge regions it can be used also to access the extended x-ray absorption fine structure. Specifically the bulk sensitivity of this technique makes experiments feasible in which complicated sample environments are needed. Hence manifold studies on liquids and solids under high pressure conditions have been accomplished. This presentation gives a short introduction to non-resonant x-ray Raman spectroscopy. The special properties of this technique will be emphasized and exemplified by discussing recent studies of liquids, complex materials and samples under extreme conditions.

Keywords: X-ray scattering, absorption spectroscopy, complex materials

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Pressure-induced structural transition in oxides at high pressure: Inelastic X-ray scattering study

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The structures of crystalline and amorphous oxides at high pressure are essential to understand their thermodynamic and electronic properties. Experimental studies of pressure-induced structural changes in the archetypal low-z oxide glasses and crystals (i.e. borates and silicates), however, limited due to the lack of suitable experimental probes. The inherent difficulties of current technologies pose major challenges for probing structural changes of low-z glasses over a wide pressure ranges. Recent progress in in-situ high pressure inelastic x-ray scattering (IXS) with advanced x-ray optics and diamond anvil cell technology, has enabled us to reveal pressure-induced structural changes in archetypal low z- amorphous and crystalline oxides. Here, we report our recent progress about IXS studies of borates and silicates at high pressure. Pressure-induced structural changes in Na-borate glasses are characterized by a single densification pathway in stark contrast to the multiple pathways shown in Li- and pure borate glasses. Oxygen, boron, and lithium K-edge spectroscopy using IXS reveals the nature of electronic bonding changes in diverse amorphous and crystalline silicates at high pressure up to 40 GPa. The result unveils the important role cation field strength plays in pressure-induced structural changes in oxide glasses. We also account for these differences with a conceptual model that utilizes pressure rigidity (the resistance to structural changes with increased pressurization) defined by the variance of the ratio of energy difference between high and low pressure states to its pressure gradient. The results and methods here give improved prospects for atomistic origins of a gradual -to an abrupt coordination transformation in amorphous and crystalline oxides.

Keywords: inelastic x-ray scattering, amorphous oxides, high-pressure

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New applications of q-dependent XRS across the periodic table

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XRS has long been discussed in an important but somewhat limited context, specifically, as a bulk-sensitive alternative to x-ray absorption spectroscopies. However, continuing developments in both experimental apparatus and theoretical methods are steadily opening up new opportunities which are special to the large momentum transfers q which can be accessed in XRS. In this presentation, we will survey a few such recent studies. These will include applications for basic spectroscopy (He gas), environmental and renewable energy (N_2 gas and $LiTiO_x$), exotic chemical bonding ($C_2B_{10}H_{12}$), and f-electron physics (CeO_2 and UO_2).

Keywords: inelastic x-ray scattering, X-ray Raman scattering, electron energy loss spectroscopy

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X-ray Raman of water in the condensed phases

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In-situ measurement of the x-ray Raman spectra on the oxygen K-edge of several forms of ordered and disordered ice will be reported. It is shown there is a significant difference in the absorption profile in the near-edge and post-edge region between crystalline and amorphous ices. Comparisons between observed and theoretical spectra are made. Difficulties in the first-principles calculation of core level absorption spectra will be discussed.

Keywords: X-ray raman, a ray absorption spectroscopy, ice

MS.94.5

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High-resolution X-ray Raman scattering and the study of ices under high pressure

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High-resolution x-ray Raman scattering (XRS) of oxygen K-edge in various forms of ices have drawn a great deal of interest recently. The double differential cross section can be shown to provide the same information as that obtained by x-ray absorption spectroscopy (XAS) when the momentum transfer is small enough that the dipole approximation is valid. For low-Z elements whose inner shells are in the soft x-ray region, XRS possesses unique advantages compared to XAS due to its inherent bulk sensitivity and good penetration depth, and is especially valuable for studies under extreme thermodynamic conditions such as high pressure. At a total energy resolution of ~300 meV at 9.89keV, studies on ices III, II, IX, VI and VII at various pressure and temperature conditions indicate that the technique provides clear spectral sensitivity to both short- and long-range structural changes of the H_2O frame work. Our studies, for example, have revealed that a diminishing intensity of the pre-edge feature provides a clear signature of proton ordering in the H_2O frame work [1]. The technique, when coupled with optical Raman and x-ray diffraction, provides also a powerful tool for understanding the chemistry in the disassociation of H_2O induced by the incident x-rays under certain (P, T) conditions [2,3]. Details of these studies will be presented and discussed.

[1] Y.Q. Cai et al., Phys. Rev. Lett. 94, 025502 (2005).
[2] W.L. Mao et al., Science, 314, 636 (2006).
[3] J.F. Lin et al., Phys. Rev. Lett. (submitted) (2008).

Keywords: hydrogen bonds, electronic structure, X-ray inelastic scattering

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Nanostructure of ancient Damascus blades

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Legends tell how Damascene blades exhibiting extraordinary properties had been manufactured following secret recipes. During the last decades more sophisticated metallurgical methods have revealed details of the microstructure of this crucible (or wootz) steel. There are indications that impurities and unconventional thermo-mechanical treatments might have an essential influence on the typical Damast pattern. Using scanning and high-resolution transmission electron microscopy, X-ray diffraction as well as micro- and nanohardness measurements we have analysed specimens of two genuine Damascus sabres, which date back to the 17th century. They were kindly left to us by the Historic Museum Berne. Significant new details of the microstructure that have been revealed during our study are nanowires of cementite Fe_3C [1-2] as well as carbon nanotubes ([3] and present work). Moreover, Fe_7C_3 has been detected which is known as catalyst for hydrocarbon synthesis and which eventually converts to Fe_3C [4]. Since carbon nanotubes have become known as forming catalytically from natural fibres [5], this sheds a new light on early reports on the addition of leaves to the crucible [6].

[1] W.Kochmann, M. Reibold, R.Goldberg,W.Hauffe,A.A.Levin, D.C.Meyer,T.Stephan,H.Müller,A.Belger,P.Paufler,J. Alloys Comp. 372(2004)L15.
[2] A.A. Levin, D.C. Meyer, M. Reibold, W. Kochmann, N.Pätzke, P.Paufler, Crystal Res. Technol. 40(2005)905.
[3] M.Reibold, P. Paufler, A.A.Levin, W. Kochmann, N.Pätzke, D.C.Meyer, Nature 444(2006)286.
[4] F.H.Herbstein, J.A.Snyman, Inorg.Chem. 3(1964)894
[5] B.Goodell, X.Xie, Y.Qian,D.Zhang,M.Peterson, J.Jellison, USPTO Serial No.60/898,884.Febr.1,2007
[6] C.Ritter v.Schwarz, Stahl u.Eisen 21(1901)209

Keywords: archaeometallurgy, nanophase systems, high-resolution electron microscopy

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Scientific contribution to archaeology: Fingerprinting the ancient Egyptian objects

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Since 1999, scientists and an archaeologist have been working side by side to seek the ancient trade network. Our goal of research is to establish the regional variability of glass and faience in ancient Near East by using the high energy SR-XRF and other methods.