temperatures and energies in dynamic fluctuations. This duality points to the fundamental issue of how mean-field behavior can describe so successfully important aspects of highly correlated electron systems.

Keywords: quantum phase transition, magnetic X-ray diffraction, high pressure diamond anvil cells

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High pressure induced charge ordering in lithium vanadate spinel

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The spinel oxide LiV_2O_4 has been attracting considerable interest as the first heavy fermion oxide [1]. Although the low temperature properties of LiV_2O_4 are in striking parallel with those of intermetallic heavy fermions, it is not clear whether their similar properties have similar origins. LiV_2O_4 has a face-centered-cubic (FCC), spinel structure, and the formal oxidation of V ion is 3.5+. Previous studies showed that LiV_2O_4 remains cubic down to low temperature and that no magnetic ordering occurs down to 20 mK, indicating that all V sites are crystallographically equivalent even at low temperatures. We found that this system shows a metal-insulator transition under pressure. The metal-insulator transition can be attributed to charge ordering of V ions, similar to one observed in AlV_2O_4[2]. EXAFS measurements under high pressure for LiV_2O_4 (vanadium K edge at SLS, up to 22 GPa) indicated that a phase transition occurs probably associated with a charge ordered state[3]. It is probable that the phase transition we observed is of the same type as that of vanadium clusters, an interesting model proposed recently[4]. Experiments performed at the ESRF synchrotron (powder diffraction function of temperature and pressure) showed also a structural transition but at lower temperatures than that inferred from EXAFS measurements, and similar to the work reported earlier by Takeda et al[5].

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Keywords: high pressure, charge order, spinel

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Pressure-induced hydration and order-disorder transition in a synthetic gismondine zeolite

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Two high pressure phases of a potassium gallosilicate with a gismondine framework (K-GaSi-GIS) were characterized using Rietveld refinements of in-situ high-pressure, high-resolution synchrotron X-ray powder diffraction data. The observed response of the K-GaSi-GIS framework under hydrostatic pressure is a gradual flattening of the so-called 'double crankshaft' structural chain units. At pressures below 1.0(1) GPa, additional water molecules from the hydrostatic pressure-transmitting medium are inserted into the potassium-water guest network ('pressure-induced hydration') resulting in a 'super-hydrated' high pressure phase I. As the flattening of the 'double crankshaft' structural units in the GIS-framework continues above 1.6 GPa, the ellipticity of the cross-linking 8-ring windows is reduced below a certain threshold and a disordering of the potassium-water guest structure along the 8-ring channel, characteristic of a disordered high pressure phase II, is observed. The concerted framework distortion and guest network disordering accommodates the increased hydration level while maintaining the seven-fold coordination environment of the potassium cations to framework oxygen atoms and water molecules. We have thus established the atomistic details of a guest-host order-disorder transition under pressure-induced hydration conditions in a zeolite with GIS-framework and compared it to other zeolites during pressure-induced hydration. We find that the structural changes mediated by the extra framework cations and their coordination environment under PIH conditions are at the core of these different mechanisms and are driving the changes in the ellipticity of pore openings, order-disorder and disorder-order transitions and framework distortions.

Keywords: zeolite crystal chemistry, high-pressure chemistry, synchrotron powder diffraction

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Lattice dynamics in incommensurate elemental crystals at high pressure

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In recent years, surprisingly complex crystal structures have been discovered in the elements at high pressures. Incommensurately modulated structures and incommensurate host-guest composite structures have been observed in various elements across the periodic table, e.g., Rb, Ba, Sc, Te, P, and I. While considerable progress has been made in determining the detailed crystal structures of these complex phases, the mechanisms of their formation and stability are not yet fully understood. Experimental data on the lattice dynamics of the complex phases will be a key ingredient to address this question, and inelastic x-ray scattering (IXS) spectroscopy is the technique of choice to study phonons throughout the Brillouin zone on samples in diamond anvil high-pressure cells. IXS experiments were performed on single crystals of the incommensurate-composite phases Rb-IV and Ba-IV as well as the incommensurately modulated phase Te-III. As a unique feature of incommensurate composite systems, two LA-like phonon branches are observed in both Rb and Ba along the direction of incommensurability, which are attributed to separate LA-type lattice vibrations in the host and guest subsystems. The host and guest sound velocities have been determined as a function of