a quantum critical point. At the present moment we are not sure what mechanism is responsible for the $E$/$T$-scaling in the magnetic quasicrystal, however, there must be interesting common background in the two seemingly different systems.

Keywords: quasicrystals, magnetic neutron scattering, magnetic structure and excitations

MS.67.3

Quantum critical points and nematics: The ruthenate $\text{Sr}_3\text{Ru}_2\text{O}_7$

Santiago A Grigera

School of Physics and Astronomy, University of St Andrews, St Andrews, Fife, KY169SS, UK, E-mail: sag2@st-and.ac.uk

$\text{Sr}_3\text{Ru}_2\text{O}_7$ is an interesting strongly correlated metal that can be tuned to show a zero temperature metamagnetic transition. In its vicinity, there is experimental evidence supporting the existence of a novel quantum phase, with anisotropic transport properties. In this talk, I will discuss this topics and describe an extensive follow-up project to characterise and understand this phase.

Keywords: magnetic phase transitions, magnetic properties, magnetic and transport behaviours

MS.67.4

Exotic superconductivity in crystals without inversion center

Youichi Yanase1, Manfred Sigrist2

1 University of Tokyo, Department of Physics, 7-3-1, Hongo, Bunkyo-ku, Tokyo, 113-0033, Japan, 2 Theoretische Physik, ETH Honggerberg, 8093 Zurich, Switzerland, E-mail: yanase@hosi.phys.s.u-tokyo.ac.jp

I am planning to talk about some exotic properties in noncentrosymmetric superconductors which have no inversion symmetry in the crystal structure. The breakdown of inversion symmetry induces:

(i) the admixture of spin singlet and spin triplet order parameters, 
(ii) helical superconductivity, 
(iii) magneto-electric effect, 
(iv) anomalous paramagnetic effect, and so on.

Our microscopic theory on the noncentrosymmetric heavy fermion materials, namely $\text{CePt}_3\text{Si}_2$, $\text{CeRhSi}_3$ and $\text{CeIrSi}_3$ will be reviewed. The possibility of $s$+$P$-wave superconductivity is pointed out. I will discuss the relationship and common physics with FFLO superconductivity in heavy fermion superconductor $\text{CeCoIn}_5$, organic superconductors, cold fermion atoms and high density quark matters.

Keywords: superconductivity, noncentrosymmetry, magnetic properties

MS.67.5

Quantum mechanical delocalization of hydrogen atoms in $(\text{NH}_4)_2\text{PtCl}_6$

Takasuke Matsuo1, Yoshio Kume2, Noriko Onoda-Yamamuro3, Osamu Yamamuro4, Akira Inaba1, Ryouji Kiyana1, Hiroyuki Kimura1, Yukio Noda1

1 Osaka University (retired), Chemistry, Graduate School of Science, Aoshinke 5 Chome 17-17, Minoo, Osaka, 562-0024, Japan, 2 Azabu University, Fuchinobe, Sagamihara, Japan, 3 Tokyo Denki University, Hiki, Japan, 4 ISSP, The University of Tokyo, Kashiwa, Chiba, Japan, 5 IMRAM, Tohoku University, Katahira, Sendai, Miyagi, Japan, E-mail: tmatsuo@bc4.so-net.ne.jp

We performed neutron diffraction on $(\text{NH}_4)_2\text{PtCl}_6$ using the JAEA single crystal diffractometer FONDER. The crystal was essentially in the ground state at 7 K. 59 (hkl) intensity data were MEM-analyzed. The resulting nuclear density is shown in the figure for the $\text{NH}_4^+$ portion of the structure. The four rings resemble the protons forming an $\text{NH}_4^+$ ion. The hydrogen atom is delocalized on the ring of ca.0.08 nm in diameter. The orientation of the $\text{NH}_4^+$ ions is thus distributed over the ring in the ground state of the crystal. The distribution is evidence for rotational tunneling of $\text{NH}_4^+$ in the cubic environment, explaining the different low temperature behavior of $(\text{NH}_4)_2\text{PtCl}_6$ and $(\text{ND}_4)_2\text{PtCl}_6$.


Keywords: proton delocalization, ammonium ion, deuterated-induced phase transition

MS.68.1

On the evaluation of energy densities with aspherical pseudoatoms: A model study

Anatoliy Volkov, Tibor Koritsanszky

Middle Tennessee State University, Chemistry, 239 Davis Science Bldg., MTSU Box 68, Murfreesboro, TN, 37132, USA, E-mail: avolkov@mtsu.edu

There is an increasing number of X-ray charge density studies reporting local and integrated kinetic-energy densities (KED) based on the pseudoatom model. These calculations utilize approximate KED functionals and invoke the local virial theorem to derive the potential-energy density. Such a procedure thus combines a formalism of limited applicability with a density model lacking a physical soundness, through a relation that is known to be valid only for the exact properties in question. The purpose of this model study is to trace the propagation of errors associated with each step of the calculation. We evaluate a number of approximate KED’s using ab initio densities and their pseudoatom representations. The results are compared with the wave-function-based KED’s locally, as well as in terms of integrated values for atomic basins. We also test theoretical densities against the local virial relationship. In line with earlier observations, our analysis shows that KED’s obtained via functionals closely resemble exact KED’s only in regions of low and flat density. The discrepancy between exact and approximate KED

Keywords: proton delocalization, ammonium ion, deuterated-induced phase transition
values at the bond critical points for covalent interactions depends on the level of theory / basis set and the polarity of the bond, and can exceed 0.15 a.u. Because of the bias in the Laplacian introduced by the pseudoatom projection, the corresponding KED values can increase by a factor of five. Detailed analysis of model data suggests that errors introduced by approximate KED functionals and those that arise due to the pseudoatom projection, fortuitously cancel each other, especially for non-hydrogen atoms. We thus tend to conclude that the analysis has little physical relevance, even if, theoretical and experimental figures appear to be in good agreement.

Keywords: charge density, kinetic energy, topological analysis

Although recent technical and methodical advances made experimental electron density determinations also on larger molecules possible, fullerenes with 60 or more atoms are still a major challenge. Their investigation is complicated by the generally poor crystal quality and by the high mobility of these molecules in the crystal lattice. That is why only a few electron density studies are reported on highly substituted C60 fullerenes, while no such investigation is known for a C70 fullerene or its derivatives until now. Here we report on three further fullerene electron density investigations. They include for the first time (to our knowledge) two C60 fullerene derivatives [C60(CF3)12]1− and [C60(CF3)14]− which have been studied based on data sets collected at the synchrotron beam lines F1 and D3 of the Hasylab, DESY. For a C60 fullerene, C60(CF3)12, crystal quality was sufficient for a high resolution data collection under home laboratory conditions (MoKα, T= 20 K). The electron densities were topologically analyzed to yield quantitatively atomic and bond topological properties, which is of special interest in the C60 case because even for free C60 the number of chemically independent atoms (na=5) and bonds (nb=8) is substantially higher than for free C60 (na=1, nb=2). In the case of C60(CF3)12, additional information about intermolecular electronic interactions in the crystal lattice was obtained which could be related to unusual physical properties of this compound such as low solubility and volatility [2]. Funding from the DFG (SPP 1188) is gratefully acknowledged.

References:

Keywords: fullerenes, C70, synchrotron radiation

Carbonyl is the most important and versatile ligand in organometallic chemistry. The reference complexes are neutral M(CO)n, where carbonyl ligands are coordinated to a zero-valent transition metal atom. However, anionic and, more recently, cationic metal carbonyl complexes have been reported and their importance in organometallic chemistry is now well recognized. Structures and properties of ionomic complexes may vary dramatically. For this reason, a quantum chemical investigation of the effects of electric field on the isolated CO molecule was undertaken, together with the analysis of chemical bonding. This allows studying the modifications of CO electron density due to coordination to the metal (separating the effects of the chemical bonding from those due to polarization). Periodic calculations were carried out on salts of ionic metal carbonyl complexes with several (hard and soft) counter-ions, with the purpose to analyze packing abilities of these species and the electron density polarization caused by the crystalline environment. For example, a species like [Co(CO)5]− was computed in known salts of Li+, Na+, K+, Rb+, Cs+, [NH(C2H5)3]+ and the newly determined salt of [N(C2H5)4]+. Similarly, [Fe(CO)5]2− was investigated as salt of [BF4]− and [SbF6]3−.