

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

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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

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Exotic superconductivity in crystals without inversion center

Youichi Yanase¹, Manfred Sigrist²

¹University of Tokyo, Department of Physics, 7-3-1, Hongo, Bunkyo-ku, Tokyo, Tokyo, 113-0033, Japan, ²Theoretische 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 CePt_3Si , CeRhSi_3 and 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 CeCoIn_5 , organic superconductors, cold fermion atoms and high density quark matters.

Keywords: superconductivity, noncentrosymmetry, magnetic properties

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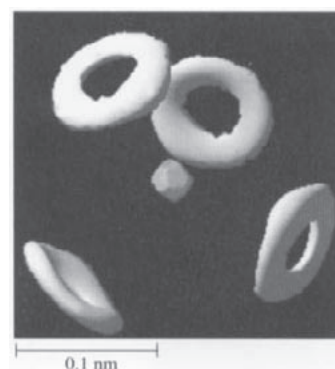
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Quantum mechanical delocalization of hydrogen atoms in $(\text{NH}_4)_2\text{PtCl}_6$

Takasuke Matsuo¹, Yoshio Kume², Noriko Onoda-Yamamuro³, Osamu Yamamuro⁴, Akira Inaba¹, Ryouji Kiyonagi⁵, Hiroyuki Kimura⁵, Yukio Noda⁵

¹Osaka University (retired), Chemistry, Graduate School of Science, Ao-Shinke 5 Chome 17-17, Minoo, Osaka, 562-0024, Japan, ²Azabu University, Fuchinobe, Sagami-hara, Japan, ³Tokyo Denki University, Hiki, Japan, ⁴ISSP, The University of Tokyo, Kashiwa, Chiba, Japan, ⁵IMRAM, 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 NH_4^+ portion of the structure. The four rings represent the protons forming an NH_4^+ ion. The hydrogen atom is delocalized on the ring of ca.0.08 nm in diameter. The orientation of the NH_4^+ ions is thus distributed over the ring in the ground state of the crystal. The distribution is evidence for rotational tunneling of NH_4^+ in the cubic environment, explaining the different low temperature behavior of $(\text{NH}_4)_2\text{PtCl}_6$ and $(\text{ND}_4)_2\text{PtCl}_6$. [1] T. Matsuo, *Pure & Appl. Chem.*, 75 (2003) 913.



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

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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

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

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Exploring pathways of structural phase transitions via experimental charge density analysis

T. N. Guru Row

Indian Institute of Science, Solid State and Structural Chemistry Unit, C.V. Raman Avenue, Bangalore, Karnataka, 560012, India, E-mail : sscnrg@sscu.iisc.ernet.in

It has been a challenge to decipher the nature of a chemical bond between two atoms in a molecule and more so to evaluate the nature of interactions between molecules/ions in a crystal. Charge density analysis has gained immense importance in recent years, particularly because such studies allow one to observe and quantify chemical bonding beyond the criteria of mere geometry [1]. The theory of "Atoms in Molecules" [2,3] has not only provided a new pathway to evaluate derived properties on the basis of charge density measurements but also allows for comparison with theoretical estimates of such densities. Recent work in our laboratory is devoted to the analysis of complex inorganic sulfates in terms of bond paths, coordination spheres, electrostatic potential surfaces and in particular to observe the changes in one electron properties and the corresponding changes in chemistry across phase transitions with temperature. A new outlook to the definition of phase transitions in terms of the nature of the chemical bond pathways is observed.

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Keywords: charge density Inorganic Materials, phase transitions, properties

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Intra and intermolecular electron density properties of fullerene derivatives: First C₇₀ examples

Peter Luger¹, Roman Kalinowski¹, Stefan Mebs¹, Manuela Weber¹, Sergey I. Troyanov², Lilianna Checinska³, Wolfgang Morgenroth⁴, Carsten Paulmann⁴

¹Freie Universitaet Berlin, Chemistry and Biochemistry/Crystallography, Fabeckstrasse 36a, Berlin, Berlin, 14195, Germany, ²Department of Chemistry, Moscow State University, 119991 Moscow, Leninskie Gory,

Russia, ³Department of Crystallography and Crystal Chemistry, University of Lodz, Pomorska 149/153, 90 236 Lodz Poland, ⁴DESY/HASYLAB, Notkestr. 85, 22603 Hamburg, Germany, E-mail : luger@chemie.fu-berlin.de

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 C₇₀ fullerene derivatives [C₇₀(C₂F₅)₁₀ [1] and C₇₀(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 (MoKalpha, T= 20 K). The electron densities were topologically analyzed to yield quantitatively atomic and bond topological properties, which is of special interest in the C₇₀ case because even for free C₇₀ 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:

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Keywords: fullerenes, C70, synchrotron radiation

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Effects of crystal packing on the electron density of metal carbonyl complexes

Piero Macchi, Davide Tiana, Angelo Sironi

University of Milano, Structural Chemistry, via Venezian 21, Milano, Milano, 20133, Italy, E-mail: piero.macchi@unimi.it

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 ionic 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)₄]⁻ was computed in known salts of Li⁺, Na⁺, K⁺, Rb⁺, Cs⁺, [NH(C₂H₅)₃]⁺ and the newly determined salt of [N(CH₃)₄]⁺. Similarly, [Fe(CO)₆]²⁺ was investigated as salt of [BF₄]⁻ and [Sb₂F₁₁]⁻.