calculate the aspherical atoms' parameters for atoms present in RNA and DNA molecules, and to enable the modelling of some other biological complexes of interest (e.g. minor groove binders). Reconstruction of the electron density enables us to perform interaction energy calculations for such systems.
Newly obtained pseudoatom models were first tested on a set of over 200 nucleic base pairs, and small charged molecular complexes. Electrostatic interaction energies were calculated for the densities reconstructed using UBDB (EPMM method) [2], and then compared against quantum calculations performed for the same systems (eg. adenine dimer, guanine-cytosine pair) at the two levels of theory *i.e.* first order electrostatic term HF/aug-cc-pVDZ and B3LYP/6-31G**. Correlation between the electrostatic interaction energy values obtained using those methods is high, while the linear coefficient is close to one. UBDB+EPMM satisfactorily reconstructs the electrostatic interaction energy, and what is particularly important, it closely reproduces the energetical trends.
The total interaction energy was estimated for the sample structures (containing DNA and RNA bases and their modifications) using the UBDB databank, and other atom-atom potential methods. Quantum mechanical interaction energy calculations (force field) were also performed. We compared all the results to get a clear idea about the accuracy and limits of all those approaches and generally to validate all available methods in this field. Good estimation of total interaction energy is very important in the potential applications of our method in the drug design and molecular biology.

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Keywords: electron density, intermolecular interactions, nucleic acids

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Hirshfeld surfaces from experimental charge density data. Radosław Kamiński, Anna A. Hoser, Krzysztof Woźniak. *Department of Chemistry, University of Warsaw, Warszawa, Poland.*
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Crystal engineering methods have recently attracted much attention due to their potential applications in predicting and designing new functional materials. Hirshfeld surfaces[1] have become a very popular tool to understand the packing of molecules in the solid state as well as intermolecular interactions between them. However, typical surfaces are defined using spherical atomic densities, which is not always the best option; especially when dealing with very accurate experimental charge density data. Thus, the whole effort to gain electron density information from the solid state is not fully utilized when applying such surfaces in the analysis. Therefore, here we propose a new approach to obtain Hirshfeld surfaces utilizing the charge density data obtained from multipole refinement with the Hansen-Coppens formalism.[2] Our methodology is tested on simple molecular examples such as, for example, α-oxalic acid dihydrate showing hidden potential of these inter-molecular surfaces.

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Keywords: crystal engineering, charge density, Hirshfeld surfaces

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Magnetoelastic coupling in the triangular lattice antiferromagnet CuCrS2 investigated by neutron and X-ray diffraction, neutron polarimetry and inelastic neutron scattering. Julia C. E. Rasch[a,b], Martin Boehm[a] ,Clemens Ritter[a], Hannu Mutka[a], Jürg Schefer[b], Lukas Keller[b], Galina M. Abramova[c], Antonio Cervellino[d] and Jörg F. Löffler[e]. [a]*Institut Laue-Langevin, 6 Rue Jules Horowitz, BP 156, FR-38042 Grenoble Cedex 9, France.* [b]*Laboratory for Neutron Scattering, ETH Zurich and Paul Scherrer Institut, CH-5232 Villigen PSI, Switzerland.* [c]*L.V. Kirensky Institute of Physics, SB RAS, Krasnoyarsk RU-660036, Russia.* [d]*Swiss Light Source, Paul Scherrer Institut, CH-5232 Villigen PSI, Switzerland.* [e]*Laboratory of Metal Physics and Technology, Department of Materials, ETH Zurich, CH-8093 Zurich, Switzerland*
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$CuCrS_2$ is a triangular lattice Heisenberg antiferromagnet with a rhombohedral crystal structure. We report
on neutron and synchrotron powder diffraction results which reveal a monoclinic lattice distortion at the
magnetic transition and verify a magnetoelastic coupling [1]. $CuCrS_2$ is therefore an interesting material to study the influence of magnetism on the relief of geometrical frustration. Polarimetry has been used to determine the magnetic structure to be a spin density wave and to exclude a helical arrangement. Because of the magnetoelastic coupling, the system is assumed to be able to select a magnetic ground state and to overcome frustration. Additionally a magnetic resonance mode has been found at $\hbar\omega$=12meV which evidences a dimerization of Cr ions in the triangular planes [2].

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On the significance of low and zero intensity observations. Julian Henn, Kathrin Meindl. *Institute of Inorganic Chemistry, University of Göttingen, Germany.*
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Counting statistics determine the minimum error present in an X-ray measurement. Thus, weak and zero intensity observations are naturally insignificant. However, a weak intensity may appear as significant by accident due to large variations in the variance of an intensity measured with low redundancy *N*. We investigate the significance of weak and zero intensity observations for the optimistic limiting case of a Poisson distribution for the individual reflections [1]. In real measurements additional sources of error are present the contribution of which even reduces the significance of weak and zero intensity observations. The redundancies required for