atoms, *i.e.* adenine- thymine (AT), guanine- cytosine (GC)- hydrogen bonding, guanine- adenine (GA)- stacking, and a group of charged species. The energetic tendencies are very well preserved, however, the energy values differ between the two methods of about 5 kcal/mol on average.

The new version of databank has also been applied to the refinement of selected nucleic acid bases and their modifications as the source of aspherical atomic scattering factors (transferred aspherical atom refinement, TAAM). It significantly improved the final geometries of molecules in the crystal, R factors and ADPs. Several other calculations were performed for the aforementioned solved structures *i.e.* periodic calculations in CRYSTAL06 [7], energy calculations with PIXEL package [8]. The results were compared to the energy values obtained with the aid of a number of force fields in order to get an idea of the accuracy and limits of all the methods [9].

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Keywords: nucleic acids, aspherical pseudoatoms, electrostatic interaction energy

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Comparison of electrostatic energies between selected DNA-ZnF complexes

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Zinc Fingers (ZnF) are small protein domains widely present mostly in *Eucaryota*. Among other structural subgroups of ZnF, the most relevant is C2H2-like family, with zinc ion tetrahedrally coordinated by two cysteine and two histidine residues. Such ZnF domain consists of 24 aminoacids folded into two anti-parallel beta-strands and an alpha-helix and recognizes DNA via hydrogen bonding with outer side of helix. ZnF can be combined with an effector domain e.g. transcriptional activator, transcriptional represor, methylation domain or nuclease. Especially ZFNs have the greatest role in molecular biology and medicine: their ability to recognize (ZnF) and cut DNA sequence (nuclease) is widely used in gene therapy.

Several structures of ZnF interacting with DNA were deposited in PDB databank. The structures with the best resolution were chosen for further studies and the UBDB databank [1] was extended with a set of new atom types.

The theoretical approach applied in this study is based on transferability of electron density parameters between atoms in chemically equivalent environments. It allows to reconstruct the unperturbated, static electron density of larger systems on the basis of experimentally obtained geometry. The electrostatic energy of interaction was calculated with EPMM method developed by Volkov [2] including Exact Potential for overlapping charge distributions and Buckingham-type multipole approximation for non-overlapping charge distributions. The quantitative characterization of particular electrostatic interactions for selected structures of interest will be presented and discussed.

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Keywords: electrostatic, protein, zinc

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Experimental charge density study and bond characterization on $[Cu(I)(4\text{-}pytH)_2](HC_4O_4)$

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TThe title compound, $[Cu(I)(4\text{-}pytH)_2](HC_4O_4)$ (4-pyt = pyridine-4-thiolate), can be obtained by the in-situ generation of 4-pytH ligand obtained from the 4-dpds (4,4'dipyridyldisulfide) precursor through the reductive cleavage of the disulfide bond of 4-dpds under solvothermal conditions. The structural analysis reveals that the tetrahedral Cu(I) ion is bonded to four sulfur atoms of the 4-Hpyt ligands forming a 1D cationic chain-like framework, $[Cu(I)(4\text{-}pytH)_2]^+$, and further extended to a pseudo-3D supramolecular architecture via the intermolecular π−π interactions and the hydrogen bonds between cation and monohydrosquarate, The Cu(I) ion is coordinated to sulfur atoms with four different Cu−S distances, 2.2458(2), 2.2793(1), 2.2983(1) and 2.8023(2)Å. A $HC_4O_4^-$ dimer is formed through two strong O−H···O hydrogen bonds with the O···O distance of 2.500 Å. The experimental charge density distribution of $[Cu(I)(4\text{-}pytH)_2](HC_4O_4)$ has been investigated in terms of a pseudo-atomic multipolar expansion (Hansen-Coppens' multipole model) using high resolution single-crystal X-ray diffraction data at 100(2) K with $\sin\theta/\lambda$ up to 1.0 and synchrotron data at 10(2) K with $\sin\theta/\lambda$ up to 1.3. The electron density will be presented in terms of deformation density as well as the Laplacian distribution. Bond characterizations are expressed in terms of topological properties associated with the bond critical points including the dative covalent Cu−S bonds and typical covalent character on N—N, N—C and C—C bonds. The detail comparison between in house and synchrotron data sets will be performed and the topological properties of those intra- and inter-molecule interactions will also be discussed in details.

Keywords: Cationic chain, Charge density analysis, Bond characterization

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MoProViewer: a molecular viewer for the MoPro charge density analysis program

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The MoPro program suite [1] is a crystal structure and charge density refinement package which includes two main modules: the MoPro least-squares refinement program and VMoPro, a tool dedicated to the computation of properties derived from the electron density. MoPro already possesses its own graphical user interface, but VMoPro was still a text-based program.

Hence we present MoProViewer: a molecular viewer designed as an interface to VMoPro, and thus especially dedicated to the field of charge density analysis. MoProViewer offers a wide range of features, among which:

- Compatibility with the MoPro molecular file format (including exportation), and with all the other formats allowed by the MoPro conversion program (CIF, shelxl RES, XD …).
- Several molecule representation modes (lines, balls & sticks).
- All standard molecular viewer capabilities (configurable atoms labeling and atoms coloring scheme, images exportation).
- All "classical" crystal structure analysis tools (stereochemistry measurements, symmetry handling, thermal ellipsoids drawing).
- Representation and modification of multipolar model atomic axis systems and chemical equivalencies constraints.
- Setup and control of most of the VMoPro possible computations (electron densities, electrostatic potentials, ρ(*r*) topology …).
- Representation of the properties computed by VMoPro, or readable in XPLOR or Gaussian CUBE format, as 3D isosurfaces, 2D isocontours plots, 3D gradient lines or 2D slices of scalar fields.
- Possibility to color any isosurface on the basis of values of any other loaded scalar field.
- Drawing of critical points and bond paths obtained from an electron density topology analysis.
- A powerful atom selection tool, which allows for instance to easily perform computation focusing on any fragments or regions of a molecule.
- Computation of the electrostatic interaction energy between two molecules in the crystal, or between any selected fragments of the loaded crystal structure.
- Handling of transferable electron density parameters database.
- Specific tools for protein structures: hydrogen atoms and water molecules handling, sequence explorer.
- Specific tool for a fast and efficient model examination in the context of a MoPro structural or charge density refinement.

MoProViewer is written in C++ and is based on the Qt SDK and on the Armadillo [2] and OpenGL libraries. It will be released as free of charge and open-source software under the GNU-GPL license.

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Keywords: charge density, molecular graphics

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Electron microscopy and x-ray diffraction study of the 1-D $(NbSe_4)_{10/3}I$ system

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The linear chain compound $(NbSe_4)_{10/3}I$ [1] shows nonlinear transport properties with a CDW transition at 285K [2]. Single crystals were examined with a four-circle x-ray diffractometer, with HREM and by measuring the temperature dependent electrical resistivity. Diffuse streaking perpendicular to the *c** direction was clearly detected in electron and x-ray diffraction patterns, both above and below the CDW transition temperature. A reversible structural transformation was observed on cooling through the CDW transition at 285K.

The RT $(NbSe_4)_{10/3}I$ structure (P4/mcc, a = 0.9464 nm, c = 3.1906 nm) is formed of $NbSe_4$ antiprisms, stacked along the *c* direction in a screw-like arrangement with 10 Nb-Se antiprisms per unit cell. Nb atoms are grouped into Nb_2 and Nb_3 segments and the Se-Se distances are correlated with the Nb chains. In accord with previous studies [3], the I atoms occupy two types of channels; those running along the [00z] direction contain four iodine atoms connected to four Se atoms, while the channels along the [11z] direction host two I atoms bonded to eight Se atoms in a square antiprismatic arrangement. Although the symmetry of the LT phase is reduced (at 100K: P2/c, a = 0.9442 nm, b = 0.9424 nm, c = 3.1883 nm and ß = 92.35º) its structure is obtained from the RT one by a minor deformation.

The electron diffraction patterns show strong diffuse streaks perpendicular to the *c** directions, confined to the (l = ±10n) layers. Additional, short and very weak diffuse streaks appear on (l = ±2n) layers. Due to the needle-like crystal morphology, the planes perpendicular to *c** direction were examined by x-ray diffraction. Reconstruction of the reciprocal space (CrysAlis software) show that the diffuse scattering observed in electron diffraction patterns at (h,k,±10n) represent projections of concentric diffuse rings. A model for the disorder in the crystal structure, based on a mismatch between the infinite $NbSe_4$ chains with random shifts along the *c* direction is proposed. A computer simulation of the disordered structure was performed for the x-ray patterns with the DISCUS package [4,5], where in addition to the shifts of the infinite $NbSe_4$ chains correlated displacements within the thermal factors were applied to the I atoms. It is shown that the disorder of the $NbSe_4$ chains is responsible for the diffuse scattering on the (h,k,±10n) planes, whereas the disorder in I positions is responsible for the weak streaking at (l = ±2n). The proposed model is used to simulate the HREM images showing defects, attributed to a precursor effect to the phase transition.

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Keywords: 1D_structure, Disorder, Diffuse_scattering

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Resonant X-ray diffraction from CB-type charge-orbital order in $Nd_{1.5}Sr_{0.5}NiO_4$

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Layered nickelate $Nd_{2-x}Sr_xNiO_4$ (NSNO) with K_2NiF_4-type structure is a rare example of a two-dimensional antiferromagnetic insulator-metal transition system, providing a contrastive counterpart to superconducting $La_{2-x}Sr_xCuO_4$ (LSCO) with the same crystal structure.