through Compton scattering, leading to highly complementary information, the momentum density . Those three functions convey distinct information, and are connected through the one particle reduced density matrix (1RDM), the key information for describing any microscopic property of a system, at least within a mean field approach. We are developing a joint analysis of those different experiments when available. It involves defining model parameterisation of the 1RDM. The method of joint refinement from independent and complementary experiments will be discussed, with applications to inorganic and molecular materials. One main interest of such approach consists in modelling condensed matter as a superposition of fragments with a flexible transferability among similar compounds. Various examples will be given, concerning inorganic complex compounds and also systems with pharmaceutical applications.
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Keywords: electron density, modeling properties, fragment transfereability

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Complex texture and structure of shocked quartz mineral with graphite grains

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Quartz mineral formed by shock impact reaction from dynamic high pressure and temperature (about several thousand degree) is still unknown so far. This paper presents detailed data with electron microscopy and X-ray structure analyses of shocked sample (SQ12 from impact crater), which are compared with normal single crystal of rock-crystal (RQ in Japan) as follows: 1) Field-emission scanning electron microscopy (FE-SEM) with analytical device indicates that shocked quartz with shocked lamellar texture (SQ12 sample) is assemblages of irregular micro-grains of 100 nm to 3 micro-meters, where carbon grains with 300 nm to 10 micrometers are involved along shocked lamellar planes, and grain-boundaries of micro-domains of quartz. 2) The EDX spectra of FE-SEM indicate that carbon grains contain some silica contents as impurities from silica-rich target rock at impact event. The present data suggest that X-ray diffraction (XRD) of powdered sample SQ12 shown as weak and diffuse X-ray intensity peaks is considered to be also effect of overlapping XRD peaks of graphite carbon. 3) X-ray structure analyses of these impact sample SQ12 compared with quartz RQ, indicates effects of irregular assemblages and shocked lamellar planes of quartz silica and graphite carbon. Structural data of shocked quartz silica formed relatively quenching process (from high-temperature and pressure) show similar data of twinning crystal data of mineral formed relatively slow-cooling process of melting. 4) Dynamic impact reaction from high pressure and temperature makes characteristic crystal data of quartz with various textures of domains, lamellae and coexisted foreign minerals as dynamic quick-cooling process.

Keywords: shocked quartz mineral, irregaular grains, graphite carbon mixing

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The effect of structural and compositional details on physical properties of new double-perovskites

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Double perovskites of general formula $A_2MM'O_6$ are a class of compounds, crystallizing in a superstructure of the perovskite type with an ordered distribution of M and M' cations on crystallographically distinct sites. The physical properties of these compounds depend strongly on details of the chemical composition and subtle structural features: Depending on the ionic radii of the M and M' ions a significant degree of cation disorder will be observed on these sites, quantified by the relative amount of M-ions on the M'-site and vice versa. A cation disorder of 0% refers to a perfectly ordered structure, while a cation disorder of 50% means a completely random distribution of the M and M' ions, representing a normal perovskite $A(M,M')O_3$. In addition to this cation disorder, oxygen vacancies can be of high relevance for the physical properties, especially if one of the elements can exist in different formal oxidation states. A very often applied approach to vary the physical properties is to substitute the A-site with another element A' with a different oxidation state and hereby changing the valencies on the M and M' sites. The interpretation of the resulting properties requires a sophisticated characterisation of the obtained material, which can only be provided by a multitechnique approach. We will report on some new examples of double perovskite compounds with A=(La^{3+},Sr^{2+}), M a 3d transition metal and M' = Ir, Ru or Re. The underlying crystal structures will be determined by several complementary methods (e.g. diffraction using synchrotron and neutron radiation, XPS, ICP-OES, oxygen determination) to resolve any ambiguity within the above mentioned structural degrees of freedom and correlate composition and structure with the resulting magnetic properties.

Keywords: perovskites, diffraction using synchrotron & neutron radiation, site disorder

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Induced structural diversity in magnetic molecular materials

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Although the basic aim of crystallography is to determine the crystal and molecular structure of crystalline solids, much more important and interesting is the relationship between structural features and physical properties. Understanding what makes a material perform its 'function' is essential for the design of new materials with novel or enhanced properties. Within this context, new opportunities for the development of novel electronic devices may arise from the