

MS12-O5**Validation and quality assessment of macromolecular structures using complex network analysis**Jure Pražnikar¹, Miloš Tomić², Dušan Turk³

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Validation of three-dimensional structures is at the core of structural determination methods. The local validation criteria, such as deviations from ideal bond length and bonding angles, Ramachandran plot outliers and clashing contacts, are a standard part of structure analysis before structure deposition, whereas the global and regional packing may not yet have been addressed. In the last two decades, three-dimensional models of macromolecules such as proteins have been successfully described by a network of nodes and edges. Amino acid residues as nodes and close contact between the residues as edges have been used to explore basic network properties, to study protein folding and stability and to predict catalytic sites. Using complex network analysis, we introduced common network parameters to distinguish between correct and incorrect three-dimensional protein structures. The analysis showed that correct structures have a higher average node degree, higher graph energy, and lower shortest path length than their incorrect counterparts. Thus, correct protein models are more densely intra-connected, and in turn, the transfer of information between nodes/amino acids is more efficient. Moreover, protein graph spectra were used to investigate model bias in protein structure.

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Keywords: macromolecule, structure validation, complex network**MS13 New insights on diffraction studies of minerals and related materials**Chairs: Dr. Catherine Dejoie,
Prof. Giuseppe Cruciani**MS13-O1****Insights into water-rock interactions in meteorites from diffraction tomography**Agnès Elmaleh¹, Jonathan P. Wright², Benoît Baptiste¹, Serena C. Tarantino³, Béatrice Doisneau¹, Erik Elkaim⁴, David Troade⁵

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Mineral hydration reactions occurred in small bodies of the solar system, likely at early stages of its history through the melting of ices accreted together with rocks, in areas located beyond the snowline. Carbonaceous chondrites, which are primitive meteorites, are witnesses of these reactions and mostly consist of hydroxylated layered silicates [1]. Their study provides understanding of the nature and stability of minerals that are important carriers of water across the solar system, and of the conditions of their formation. In carbonaceous chondrites, minerals formed during water-rock interactions present a large range of sizes (from several microns down to a few nanometers) and of compositions. In particular, the diversity of the compositions of layered silicates, mostly serpentines, exceeds by far that of terrestrial ones, including Fe and Al-rich end members; characterizing their structure is challenging because of their sub-micron size, heterogeneity and order-disorder pattern [2]. We will present results obtained by synchrotron X-Ray Diffraction Computed Tomography (XRD-CT [3]) on a series of carbonaceous chondrites of the CM family, which are carbon and hydrogen-rich chondrites in which the relatively good preservation of primary minerals allows for the reactions of hydration to be studied. We will show that varying the size of the focused beam down to 100 nm and in combination with absorption tomography, it is possible to map the distribution of hydrated nanometer-sized minerals that are difficult to characterize even by TEM, to highlight their relationship to primary anhydrous phases, and to obtain high resolution powder XRD patterns and single crystal XRD data of serpentines. Finally, we will show preliminary results of the integration of structural data and crystal-chemistry (composition, Fe valence state) of chondritic serpentines, aiming at better understanding their mixing properties along the Fe²⁺-Fe³⁺-Al³⁺-Mg²⁺ solid solutions.

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MS13-O2

Synchrotron X ray powder diffraction for the study of cutting edge zeolites applications

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Among the tectosilicates family, zeolites - of natural and synthetic origin - are certainly one of the most interesting one. Thanks to their peculiar microporous structure and chemistry, they have been widely used as highly efficient catalysts, adsorbents, and ion exchangers in petrochemical industries and in our daily life [1]. Beyond these traditional applications, recently zeolites are playing an increasingly important role in diverse areas, ranging from the environmental protection [2] to the advanced technological fields [3]. In particular, zeolites have found promising applications in the fields of renewable energy and environmental remediation, such as solar energy transport, thermal energy storage, CO₂ capture and water, soil treatment, etc. These applications make zeolites potential candidates as solutions to the sustainability issues in our society. This contribution will review some recent studies on the development of hybrid supramolecular structure (dyes/zeolite) suitable in Förster resonance energy transfer sensitized solar cell and luminescent solar concentrators and the use of high silica zeolites as adsorbent of emerging organic contaminant (ECOs) such as pharmaceutical active compounds and pesticides. Synchrotron X ray powder diffraction combined with other experimental techniques (infrared, UV-vis spectroscopy and liquid chromatography, etc.) and theoretical modeling—can be efficiently exploited to realistically localize the guest molecules in the zeolite pores. This multidisciplinary approach is of fundamental importance for the interpretation of the host –guest interaction at the base of the molecular organization and adsorption mechanisms.

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