MS19. Topology of crystal structures

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MS19-O1 Topological properties of crystal structures: from description to prediction

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Topological methods become more and more popular in crystal chemistry and materials science. At present, many topological descriptors are used to characterize and classify crystal structures. Here we consider the most important descriptors that feature local and overall architecture of the periodic networks. We mention the methods, software and databases that are used for the topological analysis and present some new ones.

However, the main purpose of the presentation is to show that the topological tools can be used not only to describe, but also to search for relations between crystal structures and to predict their topological motifs. With examples of molecular crystals, coordination polymers and intermetallic compounds we demonstrate how a knowledge database containing correlations 'chemical composition – local topology – overall topology' can be built from the initial experimental data. This database can then be used in an expert system to list possible local environments for a given structural unit (supraclusters) as well as possible extended architectures that can be assembled from the supraclusters. The probabilities of appearance of the corresponding topological motifs can be estimated that can essentially help in generation of trial structures for the subsequent evaluation by the DFT methods. Thus the topological tools being qualitative or semi-quantitative can be involved in the design of new crystalline materials in combination with the quantitative methods of mathematical modeling.

The work was supported by the Russian government (Grant 14.B25.31.0005).

Keywords: Topological methods, molecular crystals, coordination polymers, intermetallics, prediction

MS19-O2 Lanthanide-organic frameworks for optical sensing and nanothermometry

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Ln^{3+}-organic frameworks (LnMOFs) are very promising materials for tackling the challenges in engineering of luminescent centres, also presenting much potential as multifunctional systems [1]. Very few other solid-state systems provide the unique opportunities of MOFs to establish relationships between structure, topology and optical properties.

Only 10% or so of MOFs are effectively microporous, exhibiting zeolite-type behaviour, and photoluminescence. The combination of porosity and light emission allows the design of intriguing new types of chemical species and temperature sensors, which I shall highlight here, namely: (i) nanoporous Eu/4,4'-(hexafluoroisopropylidene)bis(benzoic acid) MOFs with anisotropic photoluminescence and magnetic properties and their application to sense ethanol in air [2]; (ii) miniaturized linear pH sensor based on a highly photoluminescent self-assembled Eu/1,10-phenanthroline-2,9-dicarboxylic acid MOF [3]; (iii) aqueous suspensions of Tb,Eu/1-4-benzendicarboxylate nanoparticles displaying an excellent performance as ratiometric luminescent nanothermometers in the physiological-temperature (300-320 K) range [4]; (iv) one of the most sensitive cryogenic thermometers (5.96%K^{-1} at 25 K) reported so far, $[(Tb_{0.914}Eu_{0.086})_2(PDA)_3(H_2O)]\cdot 2H_2O$ (PDA=1,4-phenylenediacetic acid), consisting of LnMOFs nanoparticles [5]; (v) post-synthetic covalent modification of IRMOF-3 followed by the coordination to Nd/Yb affords unusual near-infrared light-emitting materials [6].

I acknowledge CICECO-Aveiro Institute of Materials (Ref. FCT UID /CTM /50011/2013), financed by national funds through the FCT/MEC and when applicable co-financed by FEDER under the PT2020 Partnership Agreement.

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Keywords: MOFs, lanthanides, structure, photoluminescencence, sensing, nanothermometry