IUCr participation in the CODATA / VAMAS Working Group on Nanomaterials

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Introduction

Nanotechnology is moving towards commercialization, yet numerous scientific questions remain unanswered. One of the most critical challenges is that there is no common nomenclature or description system for nanomaterials that is accepted by a single discipline, let alone by all disciplines. The International Union of Crystallography (IUCr) and its Committee for the Maintenance of the CIF Standard (COMCIFS) are well matched to help with this task set up under the aegis of CODATA/VAMAS.

IUCr was invited to participate in a CODATA/VAMAS Working Group in 2012. CODATA is the Committee on Data for Science and Technology of ICSU, the International Council for Science (http://www.codata.org). VAMAS is the Versailles Project on Advanced Materials and Standards (http://www.vamas.org). There have been 3 Workshops so far.

The overall goal is to define the needs of as many scientific disciplines and user communities as possible. This White Paper will be transmitted to ISO Technical Committee 229 on Nanotechnology (http://www.iso.org/iso/iso_technical_committee?commid=381983) as well as other international and national standards development bodies and government agencies. Within this Working Group, crystallographers unambiguously define and characterize the structure of nanomaterials.

Crystallographic Techniques

Diffraction (scattering + interference): X-ray, gamma radiation, neutrons, electrons

Reflectivity (specular, off-specular): X-rays and neutrons

Small-angle scattering: X-rays (SAXS), neutrons (SANS)

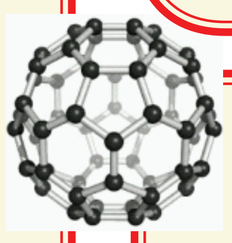
Tomography (absorption or phase contrasts): X-rays, neutrons, electrons

Imaging (HRTEM)

Spectroscopy: X-ray (XRF, XANES, EXAFS, DAFS)
electrons (EDS)
muons (μSR)
photoluminescence
dynamic light scattering (DLS)

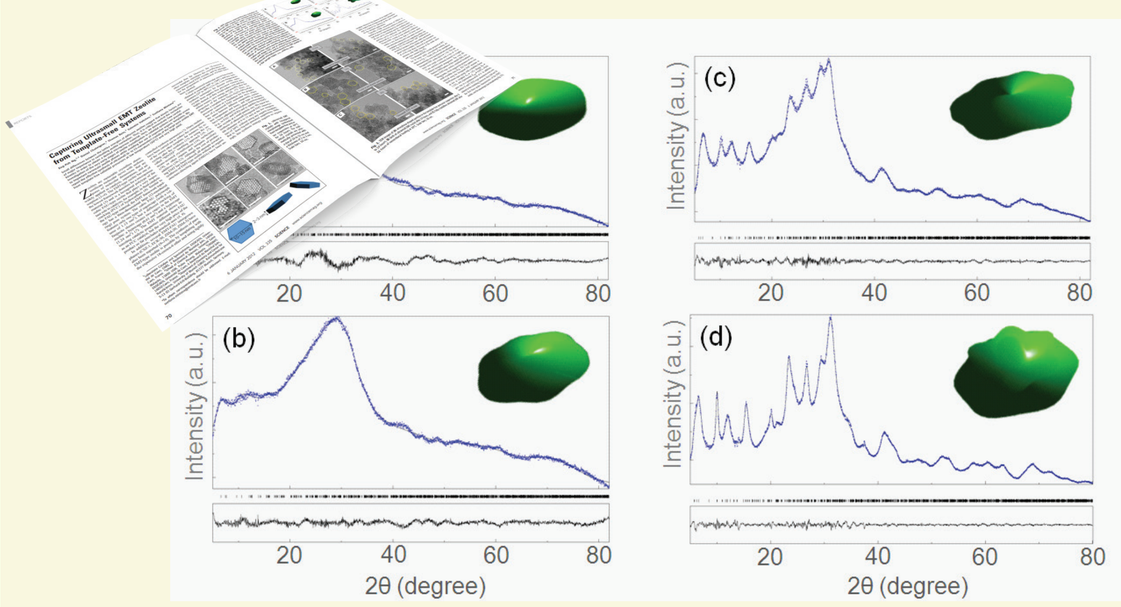
Electron, neutron and X-ray scattering and diffraction, at small and wide angles, and imaging techniques offer a physically grounded determination of the coherent size domains (including crystal shape). Our tools can approach the physical state of nanoaggregates.

Furthermore X-ray reflectivity is suitable when the nano character is only expressed along one direction (stacks, films). Compared to other fields of science, Crystallography appears as a potential leader of quantitative nanomaterial descriptors and definitions. We bring different perspectives to the task including the physical and biological sciences relevant to inorganic, organic and bio nanomaterials.



Capturing Ultrasmall EMT Zeolite from Template-Free Systems

E.-P. Ng, D. Chateigner, T. Bein, V. Valtchev & S. Mintova (2012). *Science*, **335**, 70-74



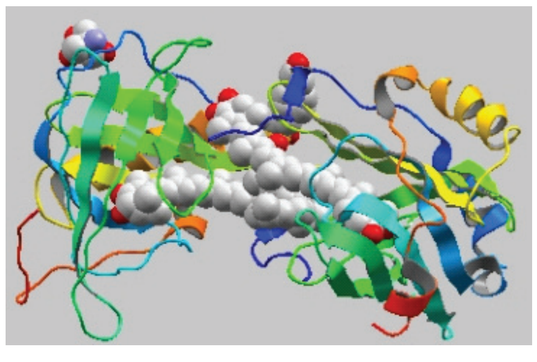
cited in *Science* Magazine 'Breakthrough of the Year 2011'

Crystallographic Information Framework (CIF)

CIF dictionaries provide a formal taxonomy of crystallographic terms and ideas. Dictionary entries are constructed in a structured machine-readable manner that facilitates validation and structuring of data: http://www.iucr.org/resources/cif/dictionaries

Dictionaries: Core, Restraints, Powder, Modulated-Composite, Electron Density, Twinning, Macromolecular, Images, Symmetry

Local dictionaries: reflectivity (to come), MPOD (properties), MAUD



Acknowledgement

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