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Topological characterization of coordination networks & metal-organic frameworks

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Coordination networks and metal-organic frameworks (MOFs) are assembled from secondary building units (SBUs) which are joined by strong chemical bonds. In the simplest cases the SBUs correspond to simple geometrical shapes such as polygons or polyhedra. In these cases the most likely (“default”) topologies are those that correspond to nets with one kind of link (“edge-transitive nets”). These and other related default structures have now been enumerated using the methods of combinatorial tiling theory [1]. These will be reviewed.

Then it will be demonstrated how the structures of MOFs can be deconstructed into nets by a systematic process that identifies the BBUs and branching points in the structure [2]. The crucial role in this process of the computer program Systre of Delgado-Friedrichs [3] in determining the combinatorial symmetry and identity of nets will be demonstrated.

The presentation will be illustrated by examples of materials with unusually interesting topologies.

[1] M. O. Delgado-Friedrichs, M. O’Keeffe and O. M. Yaghi *Phys. Chem. Chem. Phys.* 2007, 9 1035-1042. [2] M. O’Keeffe and O. M. Yaghi, *Chem. Rev.* in press. [3] O. Delgado-Friedrichs and M. O’Keeffe *Acta Crystallogr.A* 2003, 59, 351-360.

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Crystallography and HIV-1 vaccine design

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Crystallography can play a critical role in drug development, as demonstrated by structure-based drug design. But what about vaccine design? Crystallography can provide atomic-level details regarding pathogen and neutralizing antibody, but an appropriate paradigm for structure-based or structure-assisted vaccine design remains to be established. At the Vaccine Research Center, we are trying to establish such a paradigm. Crystal structures of the HIV-1 gp120 envelope glycoprotein – the primary target of neutralizing antibodies – reveal overlapping mechanisms of immune evasion [1]. These evasion tactics appear to delay the development of effective neutralizing antibodies in HIV-1 infected individuals. Such antibodies, however, do develop in 15-25% of HIV-1-infected individuals after several years.

Structures of antibodies, capable of effectively neutralizing HIV-1, reveal sites of vulnerability on the HIV-1 viral spike to antibody-mediated neutralization [2]. Neutralizing antibodies have a variety of characteristics, but virtually all of them appear to have elevated levels of affinity maturation.

Because appropriate maturation appears to be a roadblock in the development of the desired HIV-1-neutralizing antibodies, we are currently applying both structural and genomic tools to gain an understanding of the maturation process. By combining multiple structures of neutralizing antibodies with deep sequencing of the antibodyomes of individuals with broadly neutralizing antibodies,

we hope to gain insight into the parameters governing antibody maturation. Phylogenetic analysis of developing antibody lineages, for example, appears to allow maturation intermediates, common to multiple individuals, to be inferred. Modified gp120s that bind to these intermediates may guide the maturation process and thereby facilitate the generation of the desired broadly neutralizing antibodies.

[1] Kwong et al. *Nature* 1998, 393, 648-659. [2] T. Zhou et al. *Science* 2010, 329, 811-817.

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Structural characterization of applied organic materials and soft matter

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The ease with which combined X-ray diffraction and small angle X-ray scattering experiments can be assembled at a synchrotron beamline has greatly contributed to structural characterization of materials. SAXS/WAXS time-resolved experiments brought new life to the study of innumerable complex materials, and also encouraged the development of very efficient table top laboratory instruments. The information obtained from in-situ experiments, combined with other techniques and special sample environments, like controlled humidity as well as magnetic or electric fields, has greatly contributed to the elucidation of the nanostructure of advanced materials.

In this presentation, the instrumentation used to study the structural evolution of soft matter as a function of temperature at a bending magnet synchrotron radiation beamline will be briefly described. The results that will be presented here deal with quite different applied organic materials. In most cases simultaneous SAXS/WAXS and temperature scanning measurements played an essential role in describing key structural properties of those materials. Polymorphic phase transitions in triacyl-glycerides mixtures extracted from native cacao-like fruits from the Amazon region are considered important information in the area of nutrition and food research and also the cosmetic industry [1]. The production of optimized novel polymeric materials used as active layers in organic electronics was possible thanks to results from X-ray scattering and other complementary techniques that revealed the structural and dynamical properties of the polymer chains that affect light emission [2]. Creating biomaterials for medical and environmental research is also a very sought-after application, and a project is under way, which started with optimization of silica hydrogel synthesis conditions for dye-enzyme encounter in a mesoporous matrix.

As a result of new tomographic X-ray techniques, the structure of diverse natural and synthetic organic materials and soft matter is now being presented in an attractive space-volume image reconstruction. Nonetheless, to understand molecular aggregation and the phenomenon of solid phase formation, quantitative structural characterization and real time in-situ experiments continue to be indispensable for material design. The SAXS/WAXS experimental platform is now well established as an essential tool for the development of the materials of the future.

[1] Silva, J.C., Plivelic, T.S., Herrera, M.L., Rucheinsky, N., Kieckbusch, T.G., Luccas, V., Torriani, I. L. *Crystal Growth & Design*, 2009, v. 9(12), p. 5155-5163
[2] Faria, GC, Plivelic, T.S, Cusiello R.F., Souza, A.A., Atvars T.D.Z. Torriani, I.L., Deazevedo, E.R. *The Journal of physical chemistry,B*, 2009, vol. 113, nº3 3, pp. 11403-11413.

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