Contribution ID: **20** Type: **Keynote**

From Crystallography to Physical Properties: What the Second Harmonic Generation Property Is Due To?

Wednesday, 14 September 2022 15:00 (30 minutes)

For many years, our research has been focused on saccharide derived Metal Organic Frameworks (MOFs) with SHG properties and their potential applications as biosensors, because of their high biocompatibility, their lack of inversion symmetry in the crystal structure that induces the SHG properties, and their attitude to complex metal cations and pull polarizable anions into the structure. Several M(sugar)_nX₂ complexes (M=Ca,Sr; sugar=D-fructose, 2-deoxy-D-galactose, ribose; X=Cl, Br, I) were synthesized and their SHG behaviors were experimentally and theoretically studied, in order to elucidate the influence of different cations and/or anions and/or sugar and/or of their different spatial disposition in the crystals on the SHG behavior [1, 2, 3, 4].
In order to better correlate the second harmonic emission with the nature and structure of the materials, theoretical calculations were carried out with two different computational approaches, that represent the two extremes in which the real crystalline powders lie. The calculated first-order static hyperpolarizability and second-order susceptibility were compared with the experimentally measured SHG intensities.
The same approach was applied to a second class of complexes, the metal porphyrinates of formula M-TPP (M=Co, Cu, Ni, Zn, TPP=5,10,15,20-tetraphenylporphirine). These compounds show a peculiar SHG behavior: the initial efficiency was very low, but surprisingly, under laser irradiation, it gradually increased reaching after few minutes a plateau at a value about fifty times with respect to the initial one. Preliminary results on the efforts to understand this phenomenon will be reported.

[1] Marabello, D.; Antoniotti, P.; Benzi, P.; Canepa, C.; Diana, E.; Operti, L.; Mortati, L.; Sassi, M. P. Non-linear optical properties of β-D-fructopyranose calcium chloride MOFs: an experimental and theoretical approach. J. Mater. Sci. 2015, 50, 4330-4341.
[2] Marabello, D.; Antoniotti, P., Benzi, P.; Canepa, C.; Mortati, L.; Sassi, M. P. Synthesis, structure and non-linear optical properties of new isostructural β-D-fructopyranose alkaline halide metal–organic frameworks: a theoretical and an experimental study. Acta Crystallogr. B Struct. Sci. Cryst. Eng. Mater. 2017, 73, 737-743.
[3] Marabello, D.; Antoniotti, P.; Benzi, P.; Cariati, E.; Lo Presti, L.; Canepa, C. Developing new SrI2 and β-D-fructopyranose-based metal–organic frameworks with nonlinear optical properties. Acta Crystallogr. B Struct. Sci. Cryst. Eng. Mater. 2019, 75, 210-218.
[4] Marabello, D.; Antoniotti, P.; Benzi, P., Beccari, F., Canepa, C., Cariati, E., Cioci, A., Lo Presti, L. Crystal structure or chemical composition of salt–sugar-based metal–organic frameworks: what are the nonlinear optical properties due to? Acta Cryst. 2021, B77, 506–514.

Primary author: Dr MARABELLO, Domenica (Università degli Studi Torino)

Co-authors: Dr ANTONIOTTI, Paola (Dipartimento di Chimica, Università degli Studi di Torino); Dr BENZI, Paola (Dipartimento di Chimica, Università degli Studi di Torino); Dr CANEPA, Carlo (Dipartimento di Chimica, Università degli Studi di Torino); Dr CARIATI, Elena (Dipartimento di Chimica, Università degli Studi di Milano); Dr CIOCI, Alma (Dipartimento di Chimica, Università degli Studi di Torino); Dr LO PRESTI, Leonardo (Dipartimento di Chimica, Università degli Studi di Milano)

Presenter: Dr MARABELLO, Domenica (Università degli Studi Torino)

Session Classification: MS

Track Classification: Investigating Molecular Crystals: Methods and Applications