

MS43-02 | CHARACTERIZING STRUCTURE, MICROSTRUCTURE AND MORPHOLOGY OF NANOMATERIALS THROUGH RECIPROCAL SPACE TOTAL SCATTERING METHODS

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Among total scattering (TS) techniques, the Debye Scattering Equation (DSE) based approach has become a valuable tool for characterizing nanomaterials with different structure, size and morphology, with all the well-known advantages associated to the use of reciprocal space methods [1]. Since the computation operates starting from real space atomistic models, structural and microstructural information can be simultaneously derived within a unified approach. Moreover, the possibility of modeling both the small- and wide-angle regions of the X-ray TS pattern, with the DSE method, taking advantage of their complementarity in terms of length scales (from the atomic to the nanometer one), offers the opportunity of detecting sophisticated nanocrystals morphologies and disentangling defects-induced peak broadening in the TS pattern, from size-induced effects [2,3].

Here, experimental and modeling aspects related to the DSE approach, along with an overview of applications, from nanosized colloidal quantum dots and perovskites up to innovative engineered nanoapatites, will be presented.

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[2] Bertolotti, F.; Dirin, D. N.; Ibanez, M.; Krumeich, F.; Cervellino, A.; Frison, R.; Voznyy, O.; Sargent, E. H.; Kovalenko, M. V.; Guagliardi, A.; Masciocchi, N. *Nat. Mater.* 2016, 15, 987-994.

[3] Moscheni, D.; Bertolotti, F.; Piveteau, L.; Protesescu, L.; Dirin, D. N.; Kovalenko, M. V.; Cervellino, A.; Pedersen, J. S.; Masciocchi, N.; Guagliardi, A. *ACS Nano* 2018, 12, 12558-12570.