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A deep-learning approach to fast classification of quantum dots size and size dispersion from total scattering data in reciprocal space

Colloidal synthesis has emerged as a powerful bottom-up approach for the preparation of semiconductor nanocrystals with narrow size dispersion, exhibiting optoelectronic properties that can be tuned by controlling their size and morphology.
Binary Quantum Dots (QDs) of the II-VI, III-V classes and ternary nanocrystals of the metal halide perovskite family, are of major interest in the field due to heir cost-effective production processes and their competitive performances in various electronic and optoelectronic applications [1].
Reciprocal-space X-ray total scattering methods based on the Debye Scattering Equation (DSE) demonstrated themselves to be a powerful approach for the atomic-to-nanometre scale characterisation of these nanocrystals and their size/surface-induced defects [2-6]. A drawback of these techniques is that they rely on onerous procedures for the development of custom-made material-oriented atomistic models.
We try to address these limitations by implementing machine learning principles into the reciprocal-space total scattering topic, specifically developed for application to colloidal nanocrystals. At this aim we propose, here, a deep-learning-based approach to predict the average size and size distribution of colloidal PbS QDs.
Taking advantage of routines implemented into the Debussy Suite program package [7], we simulated by the DSE the total scattering patterns of PbS QDs characterized by different sizes, size distribution and lattice strain.
We then applied a physic-informed data augmentation to the simulated patterns, in order to take into account real sample features, such as different signal-to-noise ratios and the presence of different solvents redispersing the QDs in colloids.
Using these synthetic data, we trained an all-convolutional neural network [8] with a supervised-learning approach and obtained a testing accuracy of ~ 95%.
Application of this method to experimental data of colloidal QDs is foreseen in order to provide the chemist and material scientist communities with an intuitive tool for the fast screening of QDs size and size dispersion, based on statistically robust data providing distribution properties of the ensemble sample as a whole.

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Primary author: Ms ALLARA, Lucia (University of Insubria)

Co-authors: Ms BERTOLOTTI, Federca (University of Insubria); Ms GUAGLIARDI, Antonietta (CNR-IC)

Presenter: Ms ALLARA, Lucia (University of Insubria)

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