Generating Machine Learning Force-Fields for colloidal Quantum Dots. The case for CdSe, PbSe and InP

Muhammad Usman[1], Ivan Infante[1,2]
[1]BCMaterials, Bld. Martina Casiano, Barrio Sarriena s/n, 48940, Leioa, Spain
[2]Ikerbasque, Plaza Euskadi 5, 48009, Bilbao, Spain

Ivan.infante@bcmaterials.net

Colloidal quantum dots (QDs) exhibit complex electronic, optical, and structural properties that are crucial for various applications in optoelectronics, photovoltaics, and nanomedicine. The development of precise and computationally efficient tools to model QDs with high accuracy is a key area of research [1].

In this work, we employ machine learning techniques to predict QD forces and energies with the same level of accuracy as density functional theory (DFT), but at a significantly reduced computational cost. This approach, particularly beneficial for larger systems, enables molecular dynamics (MD) simulations to be extended to timescales that were previously unattainable with DFT.

Large datasets derived from reference DFT-based MD simulations are used to train machine learning models, which provide accurate predictions of interatomic forces and energies. The resulting ML-driven force fields effectively replicate key structural characteristics of colloidal QDs, especially in the surface region, and their performance is rigorously validated against theoretical predictions and experimental observations [2].

In this study, I present a diverse range of nanostructural combinations, including CdSe, InP, PbSe, and $CsPbBr_3$ QDs, trained using ML-based force fields. The findings underscore the critical role of machine learning in advancing our understanding of QD behavior under various experimental conditions, including their synthesis environment and their application in optoelectronic devices such as thin films. This work highlights the transformative potential of integrating machine learning into the computational toolkit for nanomaterial design.

Figures

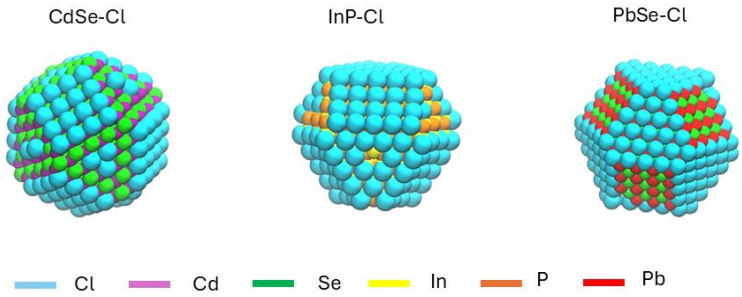

Figure 1. Illustration of quantum dot (QD) structures

References

[1] F. P. García de Arquer, D. V. Talapin, V. I. Klimov, Y. Arakawa, M. Bayer, and E. H. Sargent, 'Semiconductor quantum dots: Technological progress and future challenges', *Science*, vol. 373, no. 6555, p. eaaz8541, Aug. 2021, doi: 10.1126/science.aaz8541.

[2] O. T. Unke *et al.*, 'Machine Learning Force Fields', *Chem. Rev.*, vol. 121, no. 16, pp. 10142–10186, Aug. 2021, doi: 10.1021/acs.chemrev.0c01111.