

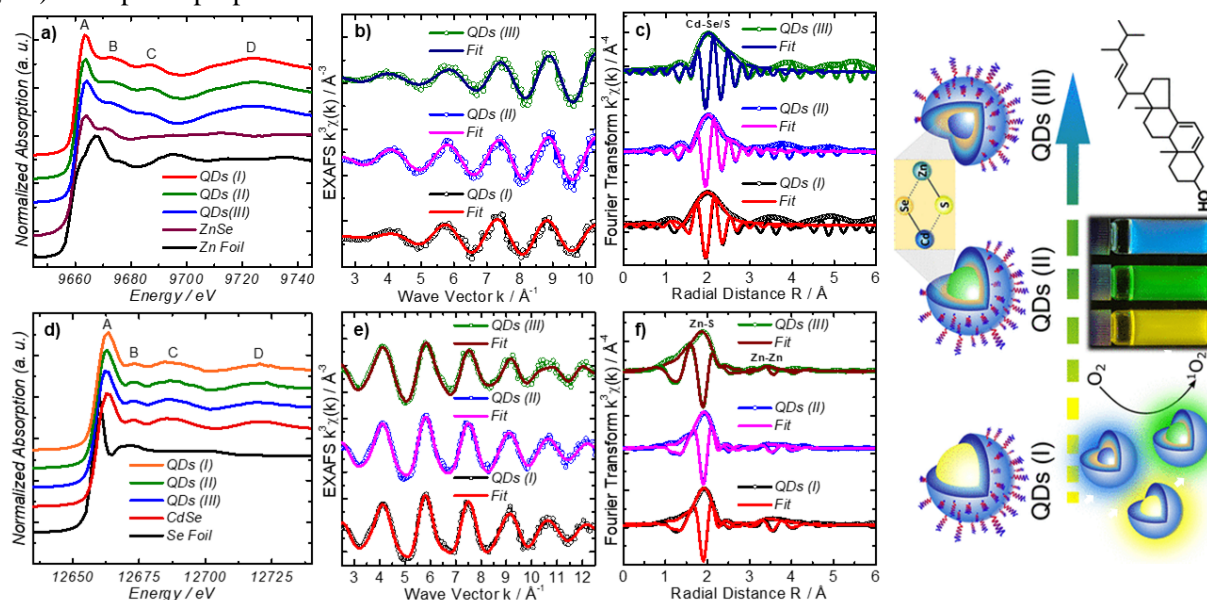
# X-ray Absorption Spectroscopy in Luminescent Materials: From Trivial Data Analysis to Machine Learning

**L.U. Khan<sup>1</sup>**

<sup>1</sup>Synchrotron-light for Experimental Science and Applications in the Middle East (SESAME) P.O. Box 7, Allan 19252, Jordan

e-mail: latifullah.khan@sesame.org.jo

The luminescent rare earths materials and quantum confined semiconductor nanocrystals are important photoemitters in visible to near-infrared spectral region, manifesting wide photonic applications in light-emitting diodes (LEDs), telecommunications, optical lasers, display devices, optical quantum memories, photovoltaic cells, night vision devices and medical diagnostics. In order to get detailed insight into the photo-physical characteristics of these materials, it is very important to probe the local atomic/electronic structure of the metal's sites. X-ray absorption spectroscopy (XAS) can be very potent to probe the metal ions, from oxidation state/electronic structure in near edge region (XANES) to the local atomic structure order around the photoabsorber in extended region (EXAFS). A crucial relation between the X-ray photon and optical photon is manifested by X-ray excited optical luminescence (XEOL), demonstrating the fundamental mechanism of the conversion of X-ray energy absorbed by the system to optical photons. XEOL is often used together with XANES to provide site specificity and reveal the electronic structure and optical properties of the wide range of luminescent materials. In present work, we present strategy based on modern data science PyFitIt machine learning package to quantitatively gain insight on the three-dimensional local structure of the luminescent materials from XANES simulation [1], in correlation with classical Continuous Cauchy wavelet transform (CCWT), conventional EXAFS fit analyses (Figure) and optical properties.



**Figure.** XANES spectra (a,d), and  $k^3$ -weighted experimental EXAFS signals and respective Fourier transforms with best fits at the Cd  $K$ -edge (26711 eV) (b,c) and Zn  $K$ -edge (9659 eV) (e,f) for the CdSe/ZnS QDs.

**Acknowledgement:** The authors acknowledge the financial support by Royal Society of Chemistry Inclusion and Diversity Fund (RSC) and BM-08 XAFS/XRF Beamline of SESAME for XAFS data measurements.

## References

- [1] L.U. Khan, Z.U. Khan, L. Blois, L. Tabassam, H.F. Brito and S.J.A. A. Figueroa, *Inorganic Chemistry*, 62 2023, 2738–2750. DOI: [10.1021/acs.inorgchem.2c03850](https://doi.org/10.1021/acs.inorgchem.2c03850)