XXI Brazilian Meeting on Inorganic Chemistry
X Brazilian Meeting on Rare Earths
III Workshop on Theoretical Bioinorganic Chemistry
Belo Horizonte, September 12 - 15th 2024

Enhancing the optical properties of hydrophilic quantum dots based on silver and indium chalcogenides by using chemometric approaches

Mércia S. Freire[1], Hitalo J. B. Silva[1], Gabriela M. Albuquerque[1], Rebeca M. Melo[1], Paulo H. Belo[1], Claudete F. Pereira[1], Goreti Pereira[1,2] and Giovannia A. L. Pereira[1]

[1]Department of Chemistry, Federal University of Pernambuco, Recife, Brazil
[2] Department of Chemistry, Aveiro University, Aveiro, Portugal
E-mail:giovannia.pereira@ufpe.br

Thematic Area: Materials Chemistry

Keywords: Ternary Quantum Dots, Aqueous Synthesis, Chemometrics.

Quantum dots (QDs) are semiconductor nanocrystals ranging from 2 to 10 nm. Due to the quantum confinement effect, these nanocrystals exhibit unique optical properties, high photostability, resistance to photodegradation and a chemically active surface, enabling a variety of applications such as sensors, solar cells, cellular probes and drug delivery systems [1, 2]. However, the QDs most studied in the literature have limited use in vivo due to the presence of heavy metals such as cadmium and lead, which are also harmful to health and the environment. This study aimed to optimize a one-pot procedure for producing hydrophilic $AgInSe_2$ and $AgInTe_2$ QDs, maximizing their emission intensity through multivariate optimization. A chemometric study was carried out to evaluate several synthetic parameters, such as reaction time, reagent molar ratios, nature of the stabilizer and reducing agent, to optimize the fluorescence intensity of the QDs. The optical results were promising, presenting a narrow and intense fluorescence spectrum, which remained stable for at least two months after synthesis. The XRD pattern revealed the presence of overlapping peaks that may be related to the crystalline structure of the QDs formed, and the FTIR confirmed the surface passivation of the nanocrystal by the stabilizer. Therefore, it is believed that it was possible to synthesize hydrophilic AgInSe2 and AgInTe2 QDs with optimized emission intensity through a chemometric approach, which are promising to be applied as optical sensors and probes.

Acknowledgments: The authors are grateful to UFPE, CNPq, FACEPE, INCTAA and CESAM/FCT/MCTES (UIDP/50017/2020+UIDB/50017/2020+LA/P/0094/2020).

References

[1] Pereira, M. G. C. et al. **Elsevier**, 2016 v. 1, p. 131-158
[2] MAY, Bambesiwe M. et al. **RSC advances**, 2022 v. 12, n. 18, p. 11216-11232.