Sessions: Nanotechnology

Preferred presentation Type: Poster

THEORETICAL AND EXPERIMENTAL STUDY OF THE ELECTRONIC AND OPTICAL PROPERTIES OF PURE KDP CRYSTAL AND Pd^{+2} DOPED KDP (Pd:KDP)

J. A. dos S. Cardoso[a], F. F. de Sousa[a], P. T. C. Freire[b], L. F. L. da Silva[c], S. G. C. Moreira[a]

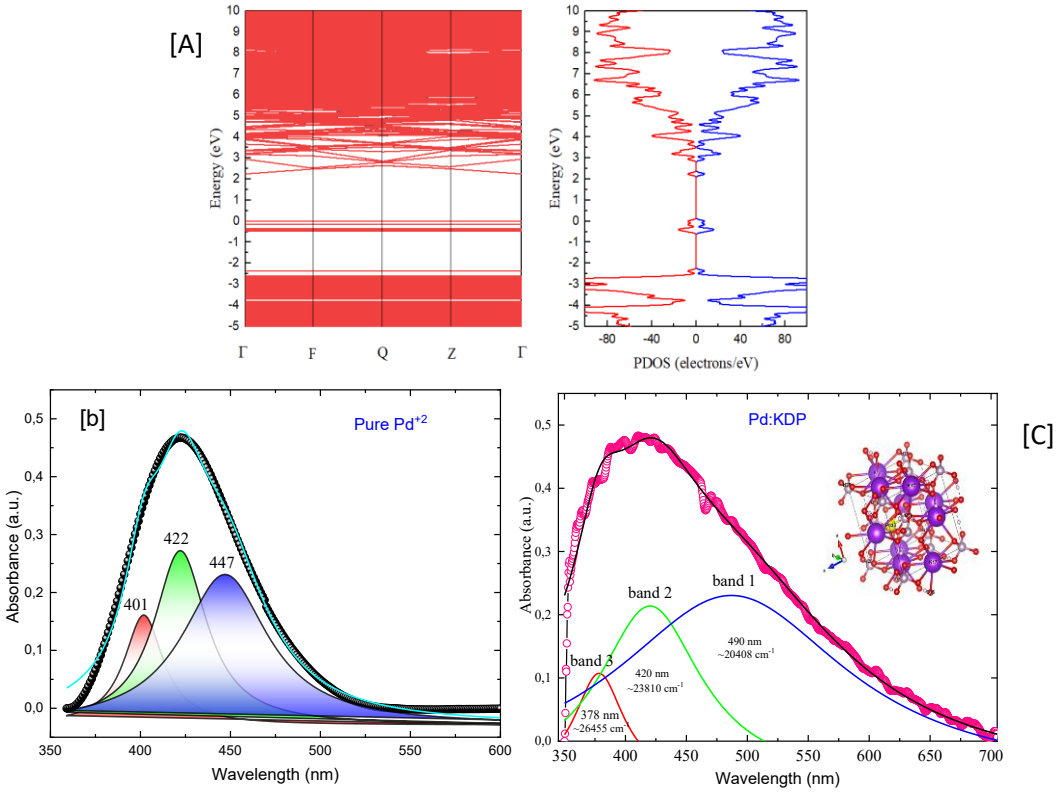
[a]Institute of Exact and Natural Sciences, Federal University of Pará, Belém, PA 66075-110, Brazil

[b]Department of Physics, Federal University of Ceará, Ceará, CE 65455-900, Brazil

[c]Institute of criminalistics, Scientific Police of Pará, Marabá 68507-000, PA, Brazil

Abstract:

This study investigates the electronic and optical properties of potassium dihydrogen phosphate (KDP) in its pure form and doped with Pd^{2+}. DFT calculations, (Figura-A) show that the band gap of KDP decreases from 5.53 eV to 2.24 eV upon doping, making it a semiconductor. The UV-Vis spectrum reveals three main absorption bands (378, 420, and 490 nm), (Figure [B-C]), attributed to metal–ligand charge transfer transitions, confirming a direct optical gap of 2.14 eV. SEM/EDS analyses highlight morphological changes and the incorporation of Pd at low concentration. The results demonstrate that Pd significantly modifies KDP, making it promising for applications in photonics, optoelectronics, and solar energy harvesting.



References:

H. J. Monkhorst and J. D. Pack, Special points for Brillouin-Zone integrations, *Phys. Rev. B* 13, 5188 (1976)

G. P. Bernd, et al, Relaxation of Crystals with the Quasi-Newton Method, *J. comp. Phys.* 131 (1997) 233–240.

A. Ioanid, UV-VIS Absorption Spectrum of the KDP:Pd System, Journal of Optoelectronics and Advanced Materials, Vol. 2, No. 3, p. 275-280, setembro de 2000.