$(ZnO)_{42}$ nanocluster: A novel visibly active magic quantum dot under first principle investigation

Bijal R. Mehta[1#], Esha V. Shah[1#], Sutapa Mondal Roy[2*] and Debesh R. Roy[1*]

[1]Materials and Biophysics Group, Department of Physics, Sardar Vallabhbhai National Institute of Technology, Surat 395007, India.

[2]Sir P. T. Sarvajanik College of Science, Veer Narmad South Gujarat University, Surat 395001, India.

[*]*E-mail address of corresponding author:* **smr@ptscience.ac.in (SMR), drr@phy.svnit.ac.in (DRR)**

Abstract

A systematic density functional investigation on the structural, electronic and optical properties of the growth of $(ZnO)_6$ cluster unit in the series of $(ZnO)_{6n}$ for n=1–9 is performed in this report. Different electronic properties of $(ZnO)_{6n}$ nanoclusters are analyzed in terms of HOMO-LUMO gap (HLG), ionization potential (IP), electron affinity (EA), chemical hardness (η) and electrophilicity index (ω) which all shows a zigzag behavior as the size of $(ZnO)_{6n}$ clusters increases[1]. The electronic energy gain (ΔE) of the clusters identified an exceptionally stable, 'magic' nanocluster, viz. $(ZnO)_{42}$. Frontier orbitals analysis results indicate easy electron transfer in $(ZnO)_{42}$ nanocluster system. The optical absorption spectra confirm that the magic $(ZnO)_{42}$ nanocluster is active in the visible range (λ=406.8 Å) of electromagnetic radiation[2]. Interestingly, like zig-zag electronic properties, similar optical switching towards the growth of $(ZnO)_6$ unit is also observed. The simulation results of electronic properties as well as the infrared spectra of magic $(ZnO)_{42}$ cluster will open up a vista to the experimentalists for its possible synthesis, which in turn will help in the development of the visibly active magic $(ZnO)_{42}$ nanocluster with novel applications in the fields of quantum dots or assembled materials.

References

1. Chen, M.; Straatsma, T. P.; Fang, Z.; Dixon, D. A. Structural and Electronic Property Study of (ZnO)n, n ≤ 168: Transition from Zinc Oxide Molecular Clusters to Ultrasmall Nanoparticles. J. Phys. Chem. C 2016, 120, 20400−20418.

2. Roy, D. R., Shah, E. V. & Mondal Roy, S. Optical Activity of Co-Poprhyrin in the Light of IR and Raman Spectroscopy: A Critical DFT Investigation. Spectroch. Acta A 190, 121-128 (2018).