Characterization of opto-electronic properties of thermally evaporated ZnO

Azmi F.F.A.[a]; Kadir M.F.Z.[b]; Aziz, Shujahadeen B.[c, d]; Muzakir S.K.[a]

[a] Material Technology Programme, Faculty of Industrial Sciences and Technology, Universiti Malaysia Pahang, Lebuhraya Tun Razak, Kuantan, Pahang, Gambang, 26300, Malaysia

[b] Center of Foundation Studies in Science, University of Malaya, Kuala Lumpur, 50603, Malaysia

[c] Advanced Polymeric Materials Research Lab, Department of Physics, College of Science, University of Sulaimani, Kurdistan Regional Government-Iraq, Qlyasan Street, Sulaimani, Iraq

[d] Department of Civil Engineering, College of Engineering, Komar University of Science and Technology, Kurdistan Regional Government, Sulaimani, 46001, Iraq

ABSTRACT

Photoelectrode plays significant role in excitonic solar cells i.e., (i) as an acceptor and (ii) transport media of excited state electron from the fluorophore upon absorption of energy of photon; which prevents from electron-hole recombination in the fluorophore. The evolution of opto-electronic properties of the ZnO upon change of size, however, receives insufficient attention from researchers. Therefore, the aim of this paper is to establish few realistic clusters of (ZnO)n (n = 3, 6, 12, 13, and 21) to study their opto-electronic properties using quantum chemical calculations at the level of B3LYP functional and lanl2dz basis set. Geometry of the clusters were optimized to the lowest energy structures; evaluated as realistic using a combination of harmonic frequency calculations, and experimental works. A device structure of cadmium selenide-based solar cell was used in the study to analyze the energy level alignment, and compatibility of the ZnO realistic clusters.

KEYWORDS

DFT; Photoelectrode; Realistic clusters; Vacuum Thermal Evaporation; ZnO

ACKNOWLEDGEMENTS

This work is funded by the Research & Innovation Department of Universiti Malaysia Pahang, and the Ministry of Education of Malaysia through the Fundamental Research Grant Scheme (RDU150111) and Postgraduate Research Scheme (PGRS190346).