Multiple Exciton Generation in MoS_2 Nanostructures: A Density Functional Theory Study

Nur Hidayati Ain Natasha Makimin, Saifful Kamaluddin Muzakir, Nur Farha Shaafi, Muhammad Zamzuri Abdul Kadir, and Ruziana Mohamed

Abstract Excitonic solar cell which fabricated using quantum confined semiconducting material that exhibits multiple exciton generation (MEG) is speculated could achieve theoretical photovoltaic conversion efficiency more than 60%. However, the expected efficiency has yet to be reached to date. Specific size and morphology of a quantum confined semiconducting material needs to be studied to determine the presence of MEG. The objective of this study is to verify the occurrence of MEG in few realistic cluster models of MoS_2 using density functional theory (DFT) calculations. Small MoS_2 nanocrystals were modelled using GaussView 5.0 software, which later validated as realistic using harmonic frequency calculations analysis executed by Gaussian 09W software. The presence of MEG in realistic models of MoS_2 nanocrystals was studied using time-dependent density functional theory (TD-DFT) calculations. The output of the work is summarized as the followings, (i) $(MoS_2)n$ with $n = 2$, 4, 6, 8 and 12 models were established as realistic, (ii) the size of the nanocrystal models are smaller than its exciton Bohr radius (ca. 1.61 nm) i.e., 0.54, 0.62, 0.95, 1.09 and 1.57 nm respectively, and (iii) all calculated MoS_2 nanoparticle models exhibit MEG. Therefore, a practical technique that could synthesize MoS_2 nanocrystals with similar structure or geometry with that of the evaluated models would materialize a device with practical photovoltaic conversion efficiency more than 60%.

N. H. A. N. Makimin · S. K. Muzakir (✉)
Faculty of Industrial Sciences and Technology, Universiti Malaysia Pahang Al-Sultan Abdullah, Lebuh Persiaran Tun Khalil Yaakob, 26300 Kuantan, Pahang, Malaysia
e-mail: saifful@umpsa.edu.my

N. F. Shaafi
Universiti Malaysia Sabah, Jalan UMS, 88400 Kota Kinabalu, Malaysia

M. Z. Abdul Kadir
International Islamic University Malaysia, Bandar Indera Mahkota, 25200 Kuantan, Malaysia

R. Mohamed
Faculty of Applied Sciences, Universiti Teknologi MARA, 40450 Shah Alam, Selangor, Malaysia

R. Abd. Aziz et al. (eds.), *Intelligent Manufacturing and Mechatronics*, Springer Proceedings in Materials 40, https://doi.org/10.1007/978-981-99-9848-7_36