Available online at www.scholarsresearchlibrary.com

Extended Abstract

Archives of Physics Research, 2017, 08 (4)
(https://www.scholarsresearchlibrary.com/journals/archives-of-physics-research/)

ISSN 0976-0970
CODEN (USA): APRRC7

Computational verification of so-called perovskite solar cells using density functional theory

Shozo Yanagida

Osaka University, Japan

E-mail: yanagida@mls.eng.osaka-u.ac.jp

So-called perovskite solar cells (PSC) are composed of PbI6 4- (MeNH3 +)4 salt, where PbI6 4- plays an essential role as an effective solar light sensitizer with keeping semiconducting property even when aligned each other. Density-functional-theory-based molecular modeling (DFT/MM) using reported X-ray crystallographic structure of PbI6 4-/MeNH3 +/H2 O salt (named FOLLIB in Cambridge Structural Data) validates that the packing unit consisting of {(PbI6 4-)9 [(MeNH3 +)2 -H2 O]2 (MeNH3 +-H2 O)2 (MeNH3 +)2 }28- should show UV/Vis absorption spectrum at λmax=424 nm (pale yellow color) as observed for the PbI64- crystal. DFT/MM of the FOLLIB horizontal aligned component, [(PbI6 4-[(MeNH3 +)2 -H2 O]2 (MeNH3 +-H2 O)2 (MeNH3 +)2 /(PbI6 4-)2)4- verifies that the component has narrow energy gap of 0.3 eV, predicting excellent semiconducting property of the PbI64- alignment with MeNH3 +. Three H2 O-free PbI6 4-/MeNH3 + aligned components, PbI6 4-(MeNH3 +)4 , [PbI6 4-(CH3 NH3 +)3]- and [PbI6 4-(CH3 NH3 +)2]2- are molecular modeled and verified to have UV/Vis spectra at λmax=570 nm, λmax=762 nm, and λmax=945 nm, respectively. Mixtures of them will be colored black, which is consistent with observable black coloration of PbI64- alignments with MeNH3+ in amorphous solute state. It is further verified that PbI6 4- undergoes van der Waals and Coulomb interactions both with electron accepting layers, i.e., nc-TiO2 in PSC of nc-TiO2/MeNH3PbI3/spiro-OMeTAD and with electron donating layer, i.e., spiro-OMeTAD in the PSC. The molecular orbital structure and electrostatic potential map verifies formation of tight interaction between them. The electron density-based alignment PbI6 4- validates unidirectional electron transport at both interfaces, resulting in high open-circuited voltage (Voc) of ~1.0 eV in PSC. In addition, the semi-conducting sensitizing layer of PbI6 4-/MeNH3 + components validates excellent short-circuited photocurrent (Jsc), and respectable fill factor of PSC. The PbI6 4--aligned solar cell will be regarded as a kind of quantum dot solar cell. Effective sensitizing components in so-called perovskite solar cells (PSC) are lead hexaiodide (PbI64−) salts of PbI64− (MeNH3+)n (n = 2~4). Density-functional-theory-based molecular modeling (DFT/MM) of X-ray crystalline structure of PbI64−/MeNH3+ salt (FOLLIB) verifies that the packing unit of FOLLIB has UV/Vis absorption spectrum at λmax = 424 nm, giving pale yellow color as complementary color. DFT/MM of the horizontal component in the FOLLIB gives narrow energy gap of 0.3 eV, verifying remarkable semiconducting property through tight alignments of PbI64− components coupled with MeNH3+. DFT/MM of the central PbI64−/MeNH3+ components verifies that the central component has UV/Vis absorption spectra with respective λmax = 570 nm, λmax = 762 nm and λmax = 945 nm, and plays an essential role as panchromatic sensitizers. In addition, their equilibrium geometric structures show slightly hypsochromic UV/Vis absorption spectra at respective λmax = 486 nm, λmax = 560 nm, and λmax = 563 nm as results of migration of MeNH3+ close to PbI64−. DFT/MM also verifies that PbI64− components align tightly to nanocrystalline TiO2 (nc-TiO2) and to spiro-OMeTAD in PSC through electron density induced by van der Waals interaction. Electron density-based alignments of PbI64− components well explain unidirectional and leakage-free electron diffusion leading to high open-circuit voltage in PbI64−-aligned solar cells. At the same time, the semiconducting and panchromatic sensitizing layer of PbI64−/MeNH3+ components contribute to excellent short-circuit photocurrent of PbI64−-aligned solar cells.

Effective sensitizing components in so-called perovskite solar cells (PSC) are lead hexaiodide (PbI64−) salts of PbI64− (MeNH3+)n (n = 2~4). Density-functional-theory-based molecular modeling (DFT/MM) of X-ray crystalline structure of PbI64−/MeNH3+ salt (FOLLIB) verifies that the packing unit of FOLLIB has UV/Vis absorption spectrum at λmax = 424 nm, giving pale yellow color as complementary color. DFT/MM of the horizontal component in the FOLLIB gives narrow energy gap of 0.3 eV, verifying remarkable semiconducting property through tight alignments of PbI64− components coupled with MeNH3+. DFT/MM of the central PbI64−/MeNH3+ components verifies that the central component has UV/Vis absorption spectra with respective λmax = 570 nm, λmax = 762 nm and λmax = 945 nm, and plays an essential role as panchromatic sensitizers. In addition, their equilibrium geometric structures show slightly hypsochromic UV/Vis absorption spectra at respective λmax = 486 nm, λmax = 560 nm, and λmax = 563 nm as results of migration of MeNH3+ close to PbI64−. DFT/MM also verifies that PbI64− components align tightly to nanocrystalline TiO2 (nc-TiO2) and to spiro-OMeTAD in PSC through electron density induced by van der Waals interaction. Electron density-based alignments of PbI64− components well explain unidirectional and leakage-free electron diffusion leading to high open-circuit voltage in PbI64−-aligned solar cells. At the same time, the semiconducting and panchromatic sensitizing layer of PbI64−/MeNH3+ components contribute to excellent short-circuit photocurrent of PbI64−-aligned solar cells.

Bottom Note: *This work is partly presented at 3rd International Conference on Electrochemistry July 10-11, 2017, Berlin, Germany*