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

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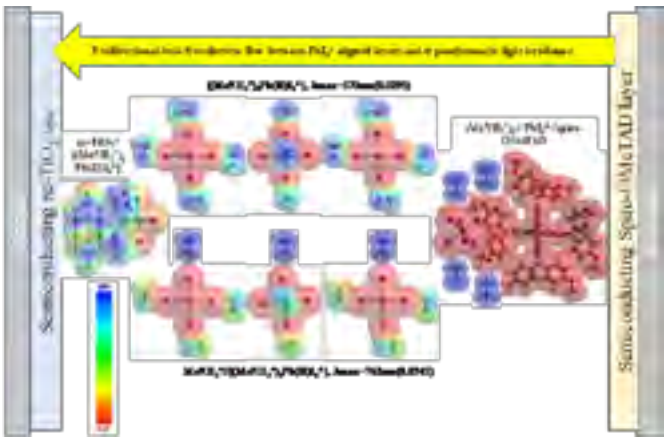
So-called perovskite solar cells (PSC) are composed of $PbI_6^{4-}$ $(MeNH_3^+)_4$ salt, where $PbI_6^{4-}$ plays an essential role as an effective solar light sensitizer with keeping semiconducting property even when aligned each other. Density-functional-theory-based molecular modeling (DFT/MM) using reported X-ray crystallographic structure of $PbI_6^{4-}/MeNH_3^+/H_2O$ salt (named FOLLIB in Cambridge Structural Data) validates that the packing unit consisting of $\{(PbI_6^{4-})_9[(MeNH_3^+)_2\text{-}H_2O]_2(MeNH_3\text{+-}H_2O)_2(MeNH_3^+)_2\}^{28-}$ 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, $[(PbI_6^{4-}[(MeNH_3^+)_2\text{-}H_2O]_2(MeNH_3^+\text{-}H_2O)_2(MeNH_3^+)_2/(PbI_6^{4-})_2)^{4-}$ verifies that the component has narrow energy gap of 0.3 eV, predicting excellent semiconducting property of the PbI64- alignment with $MeNH_3^+$. Three $H_2O$-free $PbI_6^{4-}/MeNH_3$+ aligned components, $PbI_6^{4-}(MeNH_3^+)_4$, $[PbI_6^{4-}(CH_3NH_3^+)_3]$- and $[PbI_6^{4-}(CH_3NH_3^+)_2]^{2-}$ 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 $PbI_6^{4-}$ undergoes van der Waals and Coulomb interactions both with electron accepting layers, i.e., nc-$TiO_2$ 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 $PbI_6^{4-}$ 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 $PbI_6^{4-}/MeNH_3^+$ components validates excellent short-circuited photocurrent (Jsc), and respectable fill factor of PSC. The $PbI_6^{4-}$-aligned solar cell will be regarded as a kind of quantum dot solar cell (figure 1).



## Biography

Shozo Yanagida is an Emeritus Professor of Osaka University and a Research Director of "Research Association for Technological Innovation of Organic Photovoltaics" (RATO) of University of Tokyo. Since he was promoted to a Professor of newly established "Koza" (research course) of Graduate School of Engineering in Osaka University (1980), he had contributed to photochemical conversion of solar energy, e.g., excellent photocatalysis of both nano-sized (quantized) ZnS and poly- and oligo-paraphenylene. When he was staying at SERI (now ENREL) as a visiting professor of Dr. A Nozik's group in 1984, he understood that organic molecules and their aggregates are kind of quantum dots themselves. He has his expertise in evaluation of dye-sensitized solar cells, i.e., molecular structured photovoltaics, and passion in improving photo-conversion efficiency and long-term durability of solar cells in view of unidirectional electron flow and electron lifetime in solar cell devices.

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