

Consequences of the Pb–S Bond Formation for Lead Halide Perovskites

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Streszczenie

Lead halide perovskites are structurally not stable due to their ionic bonds. Using sulfur agents in the crystal growth improves the stability and performance of the photovoltaic and light-emitting devices. In this theoretical work, we use a small toy S-radical in place of A cation in the bulk of lead iodide perovskite, and highlight the significance of the Pb-S covalent-double-bond formation for: the charge redistribution on the neighboring bonds that also turn to be covalent, phase transformation to a stable non-perovskite structure, and superior optoelectronic properties. The chemical analysis was performed with the Quantum Theory of Atoms In Molecules (QTAIM) and Non-Covalent Interactions (NCI) index. Excitonic properties were obtained from the solution of ab initio Bethe-Salpeter equation. Presence of the spin-orbit coupling triggers an interplay between the Frenkel and charge-transfer multiexcitons, switching between the photovoltaic and laser applications. Multiexcitons obey the exciton-fission preconditions.

Słowa kluczowe

lead halide perovskites, solar cells, phase transitions,
multiexcitons, singlet fission, Bethe-Salpeter equation

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