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$CH_3NH_3PbI_3$ and $CsPbI_3$ Supramolecular Clusters in 1D: Do They Evolve with the Same Principle of Cooperative Binding?[1] ARPITA VARADWAJ, PRADEEP R. VARADWAJ, KOICHI YAMASHITA, Univ of Tokyo — Development of novel semiconductor-based photo-catalytic and –voltaic systems is a major area of research in nanoscience and technologies, and engineering. The process can be either direct or indirect in converting the light energy into electricity. Some of the photovoltaics include the organic, dye-sensitized, and halide perovskite solar cells, among others. Methylammonium lead iodide ($CH_3NH_3PbI_3$) inorganic-organic hybrid perovskite is one among the many highly valued semiconductors reported till date, comparable with the inorganic cesium lead iodide ($CsPbI_3$) perovskite. These are competitive candidates in the solar energy race. Nevertheless, this study was concentrated on the fundamental understanding of the rational designs of the $CH_3NH_3PbI_3$ and $CsPbI_3$ supramolecular materials using first-principles calculations, emerged though the self-assembly of the respective building blocks. It therefore addresses the question whether the $(CH_3NH_3PbI_3)_n$ and $(CsPbI_3)_n$ (n=1–10) supramolecular clusters are the consequences of additivity, or non-additive cooperative binding? For addressing this question, the supramolecular properties such as the polarizability, the intermolecular charge transfer, and the binding energy, etc., all w.r.t the cluster size n, are exploited.

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