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**Are The Chemical Bonding Interactions in Halide Perovskite Solar Cells Cooperative?** PRADEEP VARADWAJ, ARPITA VARADWAJ, KOICHI YAMASHITA, Univ of Tokyo — Designing novel photo-sensitive and – responsive light harvesting solar cell materials is an important area of nanoscience and technologies mainly because these can transform the light energy directly or indirectly into electricity. Examples of a few of them, *inter alia*, include dye-sensitized solar cells, organic solar cells and halide perovskite solar cells. Methylammonium lead iodide ( $\text{CH}_3\text{NH}_3\text{PbI}_3$ ) organic-inorganic hybrid perovskite is one of the highly valued photocatalysts reported till date, which is comparable in its strength with the inorganic cesium lead iodide ( $\text{CsPbI}_3$ ) perovskite solar cell especially for energy conversion. The study thus has focused on the fundamental understanding of the geometrical, electronic and energetic properties of the  $\text{CH}_3\text{NH}_3\text{PbI}_3$  and  $\text{CsPbI}_3$  nanoclusters, obtained using density functional theory calculations. The main aim towards this end was to uncover the consequences of additivity, or non-additive cooperative binding, in the intermolecular chemical bonding interactions examined for these nanoclusters. The results obtained are compared with the current state-of-the-art, and will be discussed in detail.

Pradeep Varadwaj  
Univ of Tokyo

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