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 (CH$_3$NH$_3$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 (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 CH$_3$NH$_3$PbI$_3$ and 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.