

Bromination Induced Stability Enhancement with Multivalley Optical Response Signature in Guanidinium $[\text{C}(\text{NH}_2)_3]^+$ Based Hybrid Perovskite Solar Cells

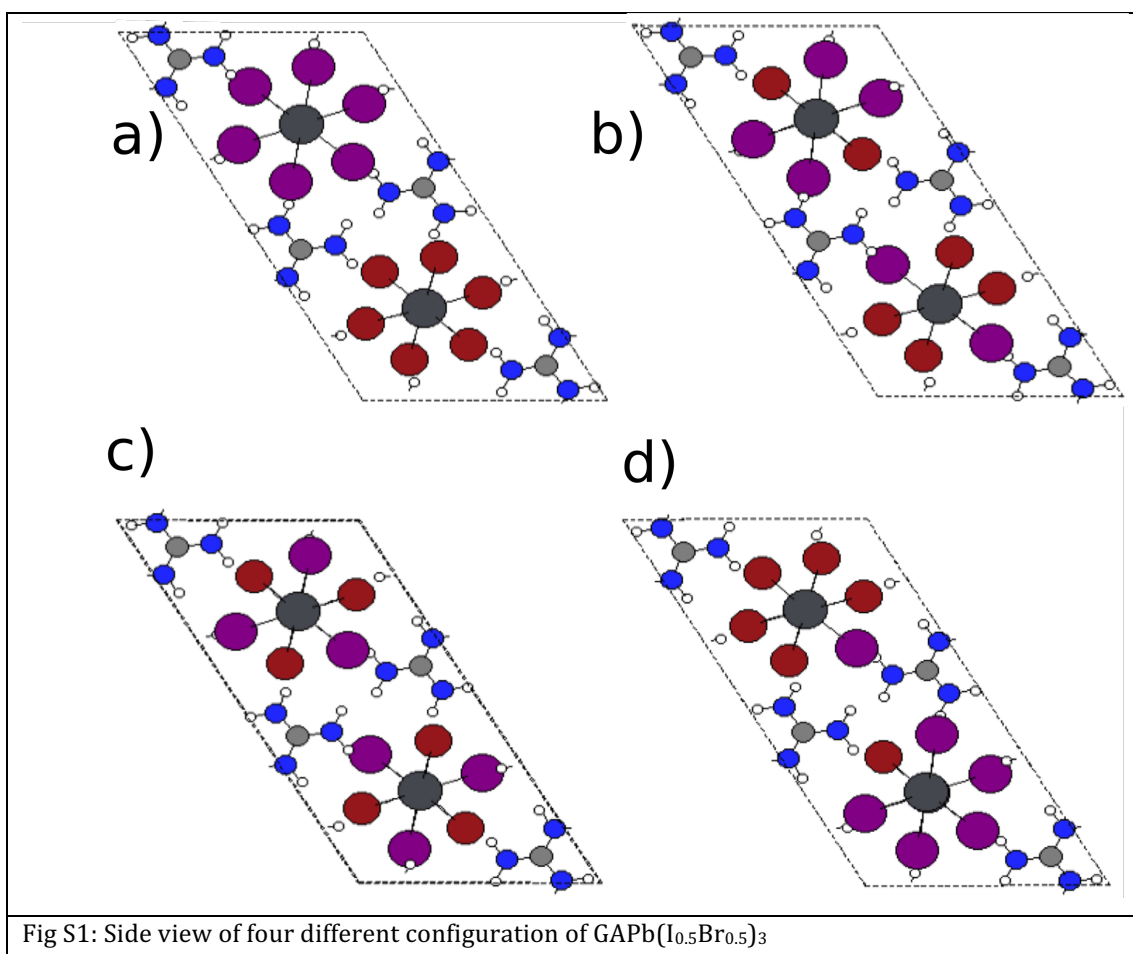
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Lowest Energy Configuration of $\text{GAPb}(\text{I}_{0.5}\text{Br}_{0.5})_3$

In case of half bromination, four different possible configurations of $\text{GAPb}(\text{I}_{0.5}\text{Br}_{0.5})_3$ are considered based on four symmetric arrangements of I and Br in Pb octahedra. The four structures are depicted in the Supplementary Information (SI), where structure A shows separate I and Br based Pb-polyhedra and mixing of different Br position with I within the same polyhedral can be seen in structure B, C and D. For the half-bromination, structure A has emerged as the stable most structure with the minimum energy configuration among four possibilities.



UV-Vis spectrum with out Spin Orbit Coupling (SOC)

