Highlights

ACTIVITY C Innovative materials with strong interplay of spin orbital charge and topological degrees of freedom-2020

Impact of local structure on halogen ion migration in layered methylammonium copper halide memory devices

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Ion migration is associated with hysteresis observed in halide perovskite-based solar cells and light-emitting diodes, however, it is crucial for their effective performance in memory devices. In the halide perovskites field, a direct link between the average/local structure and the preferred ion migration hopping pathway has yet to be established.
Adopting a combined study of average/local structural characterization and detailed electrical measurements, we shine light on the interrelationships between structure and efficiency of ion migration in layered methylammonium copper halide materials (MA_2CuX_4). In our experimental investigation, we observe that the presence of mixed Cl/Br anions not only influences the optical band gap and thermal stability but also induces intricate local structural changes that affect the ion migration and, consequently, the ON/OFF ratio in the memory devices. Through comparing the structural data obtained by detailed XRPD-PDF analysis and our devices performances, we identify several favorable conditions for halogen ion/vacancy mobility These experimental results made on single crystalline samples highlights the need to study detailed structural factors that could affect ionic migration in perovskite and perovskite-related compounds, which is important for the performance of memristor and optoelectronic devices.

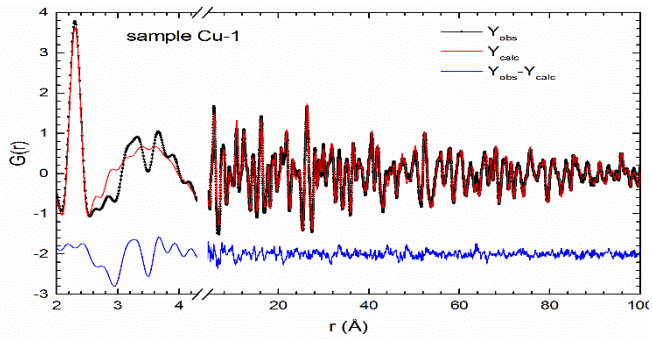

Fig. 1: Fitting of the experimental X-ray PDF function of MA_2CuCl_4.

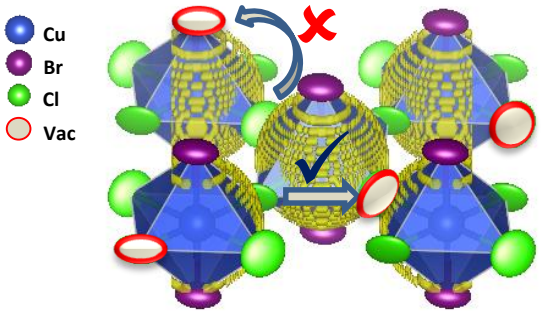

Fig. 2: Preferred migration pathways for halogen ions in Br-substituted MA_2CuCl_4 (as obtained from bond valence sum maps calculated by using XRPD and PDF data).