Phase transitions and electric dipole moments in hybrid halide perovskite single crystals

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Halide perovskites AMX_3 (A^+ = Cs, CH_3NH_3 or $HC(NH_2)_2$, M^{+2} = Pb, Sn or Ge and X^- = Cl, Br or I), are amongst the leading emerging materials in the past decade towards optoelectronic and environmental remediation applications, including devices such as solar cells, light-emitting diodes, hard radiation detectors and photocatalytic modules. What makes these semiconductor materials so attractive for optoelectronic devices is their superb absorption across the visible and near-infrared region (E_g = 1.1-3.0eV) and their high charge-carrier mobility and long charge-carrier diffusion lengths. An important research branch of halide perovskites focuses in the understanding of the underlying physicochemical origins of these fascinating properties, which is currently lacking. Such understanding will be beneficial not only from the fundamental science perspective but also crucial for the rational enhancement of the optoelectronic performance.

In this work, single-crystals of $CH_3NH_3PbX_3$ (Figure 1) were grown using a wide variety of growth techniques, from solution supersaturation and non-solvent vapor diffusion to inverse temperature growth, while the response of the electric moments of the crystals were studied with dielectric spectroscopy. All the studies were performed on well-faceted, mm-sized crystals, painted with gold electrodes. High-precision capacitance measurements were undertaken with a custom-made probe station, operating in the 80-320 K temperature range, utilizing an AC excitation voltage in a broad frequency range (f= 20Hz-2MHz). The measurements on single-crystalline specimens offer significant benefits in terms of device responsivity, because of the higher charge-carrier mobility and electrical contact uniformity. [1] AC current measurements permit investigating both the impact of the electric field stimulus on the lattice dynamics, as well as the lattice relaxation dynamics correlated with the consecutive structural phase transitions (140< T< 170 K) emerging when the materials are cooled to lower temperatures. [2]

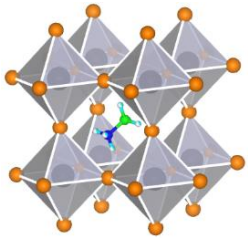

Figure 1. Crystal Structure of $CH_3NH_3PbX_3$.

References

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