Poster Presentation

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Freezing of ring-puckering molecular motion in a hexagonal perovskite compound

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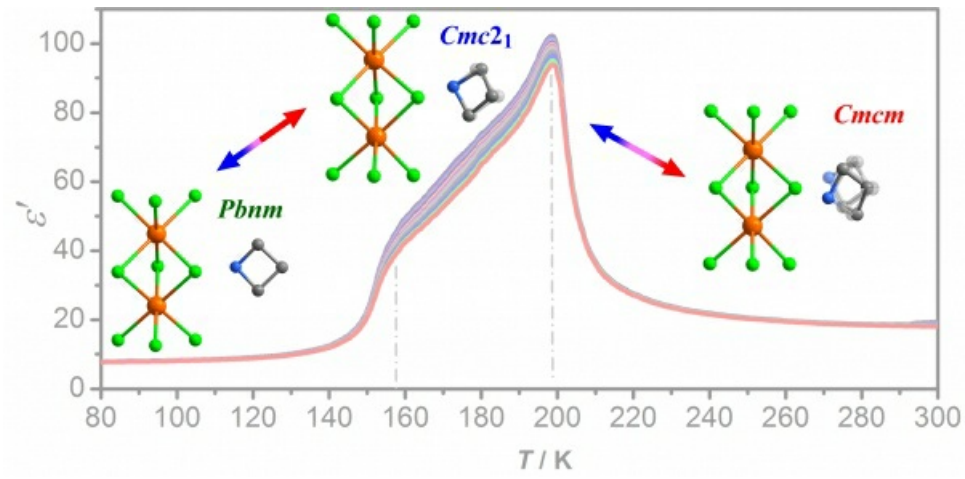
Solid-state structural phase transitions, which are induced by external stimuli such as temperature, pressure, light, and electric or magnetic fields, as a critical phenomenon, not only have fundamental significance in theoretical studies but also impart some special functions to materials, such as ferroelectric, ferroelastic, and second harmonic generation (SHG) properties, positive-to-negative thermal expansion, etc.[1] Recently, we have reported a hexagonal perovskite compound, [C4H10N][CdCl3], which is the first example of two-step nonlinear optical (NLO) switches with genuine "off–on–off" conversion between one NLO-active state and two NLO-inactive states with a remarkable "on/off" SHG contrast of ~8.0.[2] To further investigate the cation template effect in hexagonal perovskite system, by embedding a flexible four-membered ring ammonium cation, (C3H8N+), into rigid inorganic chains, we obtained a new hexagonal perovskite compound, [C3H8N][CdCl3]. Systematic characterizations including differential scanning calorimetry measurements, variable-temperature single-crystal X-ray structural analyses and dielectric measurement have revealed [C3H8N][CdCl3] undergoes two-step reversible structural phase transition at around 164 and 200 K with a space group change Pbnm ↔ Cmc21 ↔ Cmcm. Freezing of ring-puckering molecular motion of (C3H8N+) cation step by step response to the paraelectric ↔ ferroelectric transition and exceptional ferroelectric ↔ antiferroelectric transition. Investigation on the dynamic behavior of organic cation in various confined space constructed by inorganic component may be a key to deeply understand structure-property in molecular perovskites.

[1] Xu W.-J. et al, (2016) CrystEngComm. 18, 7915–7928.
[2] Xu W.-J. et al, (2016) Adv. Mater. 28, 5886-5890.



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