MS13 Structural Characterization of Functional Materials

MS13.1-05

Pressure induced phase transition in the ferroelectric hybrid perovskite $(C_6H_{11}NH_3)_2[PbBr_4]$

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Abstract

Organic-inorganic hybrid perovskites have recently emerged as highly efficient optoelectronic materials, and are being intensively investigated and developed for high performance photovoltaics, photodetections, light-emitting diodes and laser devices. Applying external pressure on hybrid perovskite materials can be used as a clean physical way to modify continuously the underlying crystal structure and consequently tune the resulting physical properties (band gap, light emission), or even generate new properties that could not be obtained at ambient conditions. Crystallographic investigations on single crystal, as a function of applied hydrostatic pressure, is in this case required to explore structure-properties relationships, and provide a clear understanding of the underlying mechanisms at the atomic level.

(C6H11NH3)2[PbBr4] is a hybrid perovskite exhibiting a 2D structural architecture with semi-conducting inorganic layers of corner-sharing PbBr6 octahedra separated by bilayers of C6H11NH3+ cations. (C6H11NH3)2[PbBr4] presents intense white light emission and ferroelectricity, characterized by a para-electric to ferro-electric transition at 360K. We have discovered that this compound undergoes a pressure induced structural phase transition, revealed by combined crystallographic and Raman studies conducted on single crystal under pressure in a diamond anvil cell. The phase transition is driven by a disorder to order phase transition of the organic framework, and proceeds without any space group change. The evolution of the unit cell parameters evidences a strongly anisotropic compressibility, in line with the low dimensionality of the structural architecture. Interestingly, the structural results indicate a stabilization of the ferroelectric phase under pressure, which opens interesting perspectives for improved performances in photovoltaics or light emitting devices.

The complete properties, including structural and vibrational ones, as a function of applied pressure will be discussed, and put in a broad perspective.

References

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