Summit to: Computational materials science

Pressure-induced indirect-direct bandgap transition of $CsPbBr_3$ single crystal and its effect on photoluminescence quantum yield

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EXTENDED ABSTRACT: Despite extensive study, the bandgap characteristics of lead halide perovskites are not well understood. Usually, these materials are considered as direct bandgap semiconductors, while their photoluminescence quantum yield (PLQY) is very low in the solid state or single crystal (SC) state. Some researchers have noted a weak indirect bandgap below the direct bandgap transition in these perovskites. Herein, application of pressure to a CsPbBr3 SC and first-principles calculations revealed that the nature of the bandgap becomes more direct at a relatively low pressure due to decreased dynamic Rashba splitting. This effect resulted in a dramatic PLQY improvement, improved more than 90 times, which overturns the traditional concept that the PLQY of lead halide perovskite SC cannot exceed 10%. Application of higher pressure transformed the CsPbBr3 SC into a pure indirect bandgap phase, which could be maintained at near-ambient pressure. We thus proved that lead halide perovskites can induce a phase transition between direct and indirect bandgaps. In addition, distinct piezochromism was observed for a perovskite SC for the first time. Our work provides a novel framework to understand the optoelectronic properties of these important materials.

BIOGRAPHY

Junbo Gong has completed his PhD at 2017 from University of science and technology of China and Postdoctoral Studies from The Chinese University of Hong Kong. He is the Asscociate researcher fellow at Wuhan University. His research interest includes CIGS and perovskite solar cells.