

# Correlative Imaging of Individual CsPbBr<sub>3</sub> Nanocrystals: Quantum Confinement Effect in Anisotropic Nanocrystals

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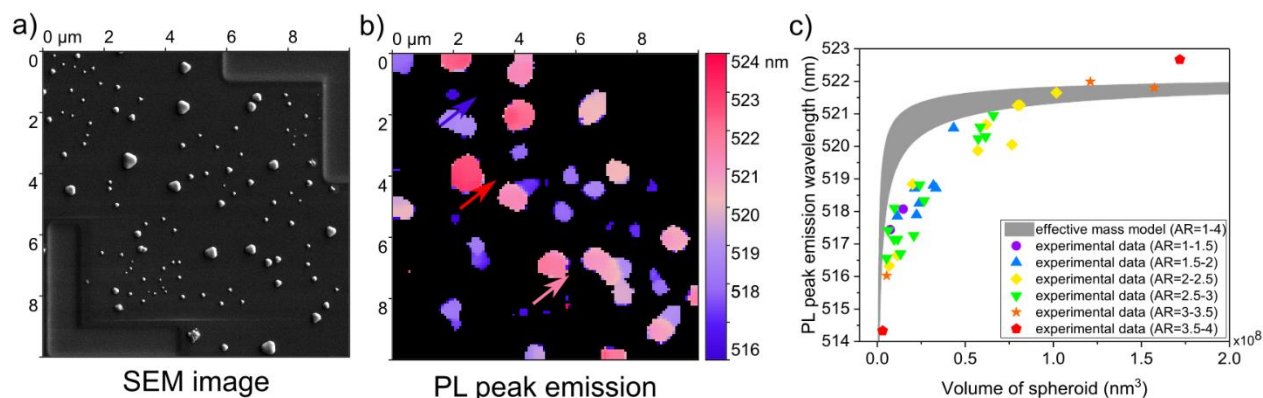
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Lead halide perovskites (LHPs) are highly promising advanced semiconducting nanomaterials with direct optical transition exhibiting bright and narrow photoluminescence (PL) tunable across the whole visible spectrum and being perspective in the field of nanophotonics, including plasmonics. Their unique optical properties and enormous optoelectronic application potential make LHPs one of the most promising class of materials of the last decade. Great benefit of LHPs in comparison to conventional semiconductors – e.g., Si or Ge – comes from the inherent ionic character which allows for cheap and simple large-scale fabrication from chemical solutions. One of the most prominent LHPs has proved to be all-inorganic LHP CsPbBr<sub>3</sub> [1-3].

The optical and electronic properties of all-inorganic CsPbBr<sub>3</sub> low-dimensional structures are strongly dependent on their morphology, size distribution and surface passivation. Decreasing the size of the CsPbBr<sub>3</sub> low-dimensional structures allows for band gap engineering or enhancing their optical properties. Moreover, colloidal CsPbBr<sub>3</sub> nanocrystals (NCs) can be prepared by hot-injection method allowing for the colloidal synthesis of well-defined, monodisperse and monocrystalline NCs with PL properties far exceeding their polycrystalline films counterparts. However, colloidal CsPbBr<sub>3</sub> NCs are extremely hard to contact due to strict metal-semiconductor junction, which significantly limits their electroluminescence performance [4]. Therefore, for the light-emitting optoelectronic applications CsPbBr<sub>3</sub> polycrystalline films or anisotropic nanocrystals are more suitable.

Here, we present a comprehensive analysis of the material PL properties of individual CsPbBr<sub>3</sub> anisotropic NCs. The individual NC analysis is possible by correlative approach based on tagging the examined area by focused ion beam and consecutive analysis by high-resolution methods – especially scanning electron microscopy (SEM) and confocal PL spectroscopy (Fig. 1a, b). We demonstrate that the PL emission of individual NCs is governed by size-dependent quantum confinement effect (QCE) predictable within a simple effective mass model which approximates the anisotropic NCs by a spheroidal shape defined by aspect ratio AR (Fig. 1c). Despite the variation in shape and dimensions of individual NCs, the observed QCE is moderate up to 9 nm in wavelength which is considerably smaller than their average PL linewidth (~16 nm). The understanding of the QCE in anisotropic CsPbBr<sub>3</sub> NCs paves a way for their integration into more complex, band gap tunable devices including optical cavities or waveguides. High PL yield of CsPbBr<sub>3</sub> together with tunable emission could be further utilized together with plasmonic resonators such as antennas or together with lattice resonances in order to create highly-efficient devices capable of engineering and controlling the light on the nanoscale.



**Fig. 1** a) SEM image of anisotropic CsPbBr<sub>3</sub> NCs correlated to the b) PL peak emission map of the identical area. The CsPbBr<sub>3</sub> NCs' shape and size are approximated by a spheroid defined by  $AR = NC's\ side\ length / NC's\ height$  and their individual PL responses are predicted based on c) the effective mass model plotted together with the experimental data.

## References

- [1] Kovalenko, M. V., Protesescu, L., Bodnarchuk, M. I. 2017. *Science*, 358, 745-750.
- [2] Rainò, G., Kovalenko, M. V. et al. 2022. *Nature Communications*, 13, 2587.
- [3] Akkerman, Q. A., Rainò, G., Kovalenko, M. V., Manna, L. G. 2018. *Nature Materials*, 17, 394-405.
- [4] Shamsi, J., Rainò, G., Kovalenko, M. V., Stranks, S. D. 2021. *Nature Nanotechnology*, 16, 1164-1168.