Lead Halide Perovskite Nanocrystals passivated with guanidinium-based ligands

Y. Berezovska[1,3], C. Bernasconi[1,3], M. Bodnarchuk[1,3], D. Dirin[1,3], A. Guagliardi[2], M. Kovalenko[1,3]*

[1]Laboratory of Inorganic Chemistry, ETH Zürich, Zürich CH-8093, Switzerland, [2]Istituto di Cristallografia & To.Sca.Lab, Consiglio Nazionale delle Ricerche, 22100 Como, Italy, [3]Laboratory for Thin Films and Photovoltaics, Empa, Dübendorf CH-8600, Switzerland

Lead halide perovskite nanocrystals (LHP NCs) exhibit immense potential for optoelectronic applications. However, due to their labile lattice and dynamic binding of ligands, they are sensitive to polar solvents and humidity. This instability hinders the processibility of LHP NCs and calls for new passivation strategies. Ligand engineering enables improved device performance and stability by enhancing charge carrier lifetime, controlling film morphology, and facilitating efficient charge transfer. Ligands with better binding groups, such as zwitterions and quaternary ammoniums, have been shown to enhance colloidal stability and LED performance. A step forward from the ammonium-based ligands can be the ligands with guanidinium fragments which exhibit excellent thermodynamic stability, high basicity, and multiple strong hydrogen-bonding capabilities.[1]

This work presents a new class of ligands with guanidinium as the binding group that were developed and used in the synthesis of LHP NCs, such as $CsPbBr_3$, $FAPbBr_3$, and $CsPbI_3$. The new synthetic approach allows obtaining LHP NCs with quantum yields as high as 95% in colloidal solutions and up to 80% in compact films. One of the ligands, Oleylguanidinium Bromide, allows synthesizing of nearly-bulk NCs with barely present quantum confinement.[2] Furthermore, these ligands enable colloidal stability in a broader range of solvents than conventional ones, which is exemplified by $CsPbBr_3$ NCs retaining high quantum yield even after two months in tetrahydrofuran.

[1] Berezovska et al., In preparation.
[2] Tamarat, P., Prin, E., Berezovska, Y. et al., *Nat Commun,* **2023,** 14, 229.