Lead Halide Perovskites: from Nanoparticles to Devices

**Background**

Perovskites are materials with a chemical formula of the form ABX$_3$, where A and B are cationic and X is anionic. Hybrid lead halide perovskites, where CH$_3$NH$_3$PbI$_3$ (methylammonium lead iodide, MAPbI$_3$) is the most notable member of the family, have been known for decades, but several recent experiments started a “perovskite fever” thanks to the dramatic increases in perovskite solar conversion efficiency seen in only a few years.

To capitalize on this, we investigate lead halide perovskites with the intention of further improving the already excellent qualities of perovskite solar cells, particularly in the areas of energy absorption, quantum yield, carrier mobility and lifetime, and diffusion length. We aimed to synthesize members of two lead halide perovskite families, CsPbX$_3$ and CH$_3$NH$_3$PbX$_3$, and examine their performance in the areas above given their prominence in the field of solar energy.

**Methods**

**Synthesis of CsPbX$_3$ nanoparticles:** Under a N$_2$ atmosphere, 15 mL of ODE, 3 mL of oleic acid, 1.5 mL of oleic acid and 0.54 mmol of PbCl$_2$ should be added to a three-neck flask. The mixture should be degassed at 100 °C for 10 minutes, mixed at 100 °C for 30 minutes (until PbCl$_2$ dissolves), and then brought to desired temperature (typically 170 °C). 0.55 mL of Cs-oleate should be quickly injected into the PbCl$_2$ solution via glass syringe through a septum. After five seconds, the three-neck flask should be cooled down by the ice-water bath. Centrifugation can extract the nanoparticles (5000 rpm, 5 min) which should then be redissolved in 8 mL of hexane. In the case of CsPbCl$_3$ and CsPbBr$_3$, 10 mL of acetic acid could be added to facilitate the precipitation.

**Crystalization of CH$_3$NH$_3$PbX$_3$:** PbX$_3$ and CH$_3$NH$_3$Br (1:1, 0.2 M) should be dissolved in N,N-dimethylformamide. N,N-Dimethylformamide single crystals should grow along with the slow diffusion of the vapor of the anti-solvent dichloromethane (DCM) into the solution.

**Summary**

Simply-synthesized CsPbX$_3$ nanoparticles can exhibit fluorescent quantum yields up to 90%, and their emission is in the visible range of spectrum with a narrow band width. The emission wavelength can be modified by tuning both size and composition of the nanoparticles, which is most easily done through the choice of halide. This makes them highly desirable for absorbing energy in solar cells, as the wide range of wavelengths covered efficiently captures a broad spectrum of solar output.

CH$_3$NH$_3$PbX$_3$ perovskites also performed exceptionally well, even relative to the highest performers in the efficiency competition. They exhibited electron mobilities up to 115 cm$^2$/Vs, diffusion lengths of up to 17 nm, and carrier lifetimes approaching 1 μs, all of which contribute greatly to pushing the boundaries of efficiency.

**References**