

STRUCTURE ANALYSIS AND EXTINCTION COEFFICIENT OF PBSE COLLOIDAL NANOCRYSTALS

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Colloidal lead selenide nanocrystals (Q-PbSe) promise to be an important material for near-infrared applications. Due to quantum confinement, their band gap can be tuned over the entire telecom wavelength range. In combination with their bright luminescence and high nonlinear refractive index, this could lead to a whole range of new applications, such as quantum dot LED's, lasers, and all-optical photonic devices.

To gain quantitative insight into the Q-PbSe optical properties, absorbance spectroscopy was used in combination with inductively coupled plasma mass spectrometry (ICP-MS). ICP-MS yields the absolute concentration of Pb and Se, from which both the Pb:Se ratio, and the concentration of the nanocrystals can be determined. The Pb:Se ratio of the nanocrystals revealed that these colloidal nanocrystals are non-stoichiometric, showing an excess of Pb atoms for all samples studied. A detailed structural model was used to confirm that this excess is located at the nanocrystal surface.

Absorbance spectroscopy on a Q-PbSe suspension of known concentration showed that we can distinguish two regions in the absorbance spectrum. Near the band gap of the nanocrystals, strong confinement effects are observed through a blue shift of the band gap with decreasing nanocrystal size, accompanied by an increase of the extinction coefficient. However, at high energies (>2.5 eV) confinement effects are no longer observed, and the extinction coefficient matches that of bulk PbSe.

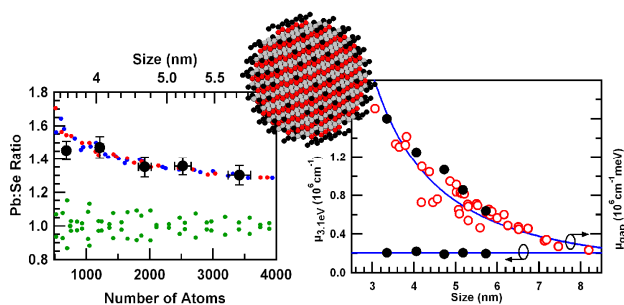


Fig. 1: Left: Experimental Pb:Se ratio (black dots), compared to a Q-PbSe model without (green dots) and with (red and blue dots) addition of surface Pb atoms. Inset: The nanocrystal model consists of a stoichiometric core of Pb (grey dots) and Se (red dots) atoms, terminated by a Pb surface shell (black dots). Right: The extinction coefficient at 400nm ($\mu_{3.1eV}$) is equal to the bulk PbSe value. At the band gap, μ_{gap} increases with decreasing Q-PbSe size, showing that smaller Q-PbSe are more efficient absorbers.