

## **Investigation of Photophysical and Electrochemical Properties of Magic-Sized CdS Nanocrystals**

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### **Abstract**

Colloidal semiconductor nanocrystals (NCs) have been the interest of many studies over the past two decades due to their applications in device fabrication, electrocatalysts, and medical diagnostics. Recent discovery of thermodynamically stable ultra-small nanocrystals (“magic-sized”) has provided the opportunity to understand their different properties at the molecular level. Herein we present the synthesis and purification of poly(ethylene glycol) thiolate-capped magic-sized CdS nanocrystals with distinct photophysical properties. These CdS NCs overcame solubility restraints by directly transferring from aqueous to organic mediums and also showed significant increased in peak sharpness when analyzed by high-resolution MALDI-TOF-MS, which confirmed formation of (CdS)<sub>33,34</sub> nanocrystals. The electrochemical properties of dissolved CdS nanocrystals were investigated in organic solvent/electrolyte medium by different voltammetric techniques. The nanocrystals displayed molecule-like HOMO-LUMO energy gap. The electrochemical features are strongly temperature, solvent, and capping-ligand thickness dependent. We also developed a working model of the energy level structure of the PEG-thiolate-capped (CdS)<sub>33,34</sub> nanocrystals.

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