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S E M I N A R

aus

Halbleiterphysik und Nanotechnologie

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"Superposition of composition and size effects in colloidal I-III-VI quantum dots"

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Composition control for I-III-VI QDs plays decisive role in tuning their optical and electronic properties. Particularly, emission efficiencies of $CuInE_2$ (E = S, Se) QDs are composition-dependent with the optimal Cu/In ratio of about 0.6.[1,2] Both concentration and distribution of Cu vacancies are important parameters for optimized $CuInE_2$ emitters. Introducing Zn into structure of ternary I-III-VI colloidal quantum dots (QDs) is known to improve their luminescence properties and environmental stability.[3] Starting from our previously reported highly luminescent Cu-In-Se (CISe) QDs,[1] we examine Zn-alloying effects for quaternary Cu-In-Zn-Se (CIZSe) QDs.

In this study, we employ a solution-processed amide-promoted approach.[4] An injection of reactive lithium- amide salt into reaction solution promotes high nucleation rates and balances the reactivity of cations. The latter allows us to precisely control the composition while keeping constant the size of colloidal QDs. We are thus able to investigate the optical properties of CIZSe QDs solely as a function of their composition. This includes the optical band gap, emission peak position, Stokes shift, and photoluminescence quantum yield (PLQY). We show that the composition for the most luminescent CIZSe QDs is around $Cu_{0.6}In_{1.2}Zn_{0.2}Se_{2+x}$. We attribute the existence of such "best-emitting" composition to a synergy of three effects – a defect ordering,[5] a structure stabilization by Zn-alloying,[3] and high concentration of In in the CIZSe structure. We then use the amide-promoted synthesis to control the QD size, which allows us to demonstrate quantum size effects for chosen Cu-In-Zn ratio in the CIZSe QDs.

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2. H. Zhong et al., *J. Phys. Chem. Lett.* **2012**, 3, 3167.
3. L. De Trizio et al. *Chem. Mater.* **2012**, 24, 2400.
4. M. Yarema et al., *ACS Nano* **2011**, 5, 3758.
5. S. B. Zhang et al., *Phys. Rev. B* **1998**, 57, 9642.