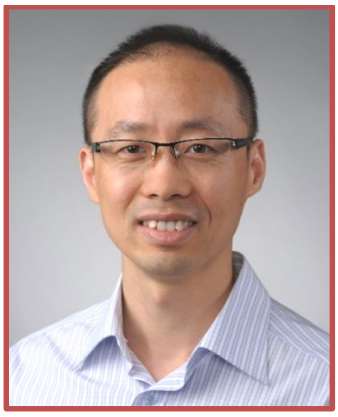
CHEMISTRY

Fall 2019 CHEMISTRY COLLOQUIA, Co-Sponsored by NCMN



October 18, 2019

3:15 Sign-in

3:30 Seminar
112 Hamilton Hall

Open to the public

Professor Weiwei Zheng
Syracuse University

From Impurities to Functionality
--- Controlled Dopant Migration Behavior in Nanocrystals

Doping of transition metal ions into semiconductor nanocrystals (NCs) is a thriving area of nanomaterials because it can introduce new optical, electronic, and magnetic properties into host NCs with broad applications in biological imaging, light-emitting devices, solar cells, photo-detectors, and quantum computing. The physical properties of a doped NCs are strongly influenced by the dopant site inside the host lattice, which determines the host–dopant coupling from the overlap between the dopant and exciton wavefunctions of the host lattice. While dopants can be introduced into NC lattice through many synthetic methods, little attention has been paid to the behavior of dopants after they have been incorporated inside a NC, or toward a mechanistic understanding of dopant behavior in the host lattice. Specifically, whether the dopant location can be modified in a controlled manner in NCs is still unknown. In our work, the effect of lattice mismatch of core/shell NCs on Mn(II) dopant behavior was studied. It was found that the dopant behavior is highly dependent upon the internal composition of the host NCs and temperature. Dopant can migrate toward the alloyed interface of core/shell NCs, which is a thermodynamically driven process to minimize the lattice strain from the cationic size mismatch between the dopant and host NCs. The dopant migration rate could be represented by the Arrhenius equation and therefore can be controlled by the temperature and lattice mismatch. Furthermore, dopant migration in the presence of lattice mismatch in core/shell NCs is identified as a new elementary process for incorporated dopants inside host NCs, which requires a lower activation energy compared to dopant ejection. Controlling dopant site by migration offers a rigorous and rational approach to design NCs with unprecedented properties, and provides new fundamental understanding of doping inside NCs as well as dopant site-dependent properties of NCs.

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