The Journal of Chemical Physics

Introduction to special issue: Colloidal quantum dots

Cite as: J. Chem. Phys. **153**, 240401 (2020); https://doi.org/10.1063/5.0039506
Submitted: 03 December 2020 . Accepted: 03 December 2020 . Published Online: 24 December 2020

Matthew C. Beard, Xiaogang Peng, Zeger Hens, and Emily A. Weiss

The Journal of Chemical Physics EDITORIAL scitation.org/journal/jcp

Introduction to special issue: Colloidal quantum dots

Cite as: J. Chem. Phys. 153, 240401 (2020); doi: 10.1063/5.0039506
Submitted: 3 December 2020 • Accepted: 3 December 2020 •
Published Online: 24 December 2020

Matthew C. Beard,[1] Xiaogang Peng,[2] Zeger Hens,[3] and Emily A. Weiss[4,a)]

AFFILIATIONS

[1]Chemistry and Nanoscience Center, National Renewable Energy Laboratory, Golden, Colorado 80401, USA
[2]Department of Chemistry, Zhejiang University, Hangzhou 310027, China
[3]Center for Nano and Biophotonics, Ghent University, 9000 Ghent, Belgium
[4]Department of Chemistry, Northwestern University, Evanston, Illinois 60208, USA

Note: This paper is part of the JCP Special Topic on Colloidal Quantum Dots.
[a)]**Author to whom correspondence should be addressed:** e-weiss@northwestern.edu

https://doi.org/10.1063/5.0039506

INTRODUCTION

The quantum confinement effect has driven the development and exploration of colloidal semiconductor nanocrystals over approximately the past three decades. These semiconductor nanostructures are typically synthesized as stable colloidal dispersions in solution-phase chemical batch reactions at relatively low temperatures. Researchers have developed a wide range of reaction conditions to produce a variety of shapes, compositions, and structures with well-controlled sizes and low polydispersities. The shape can be controlled to produce confinement in one, two, or all three spatial dimensions, the latter defining a "quantum dot." Combining two or more semiconductors within the various nanostructures produces additional optical and electronic degrees of freedom. These mixed compositional nanostructures have properties not accessible in bulk semiconductor systems. Researchers have fabricated novel nanoheterostructures, such as "dot-in-rods," quantum wells, core/shell structures, giant-core/shell tetrapods where the core is one material and the arm is another, Janus structures that consist of spherical structures with well-defined internal heterostructures, nano-dumbbells, hollow-core structures, and many other novel and interesting structures. The structural variations are seemingly only limited by the creativity of the various researchers engaged in these endeavors.

An important feature of these colloidal nanostructures is the organic molecules that decorate their surfaces, and the surface chemistry of these structures has been a constant and ongoing research topic. Much of the structural variety listed above is produced by careful control of surface interactions. For example, growing anisotropic shapes (rods, platelets, . . .) typically result from preferential binding of one surfactant molecule to a particular facet, thereby blocking its growth and allowing other facets to grow. Beyond controlling growth kinetics, the ligand/core interactions have a large impact on the resulting electrical and optical properties of the nanocrystal. For example, organic ligands can bind to dangling bonds and electronically passivate traps or otherwise defective sites leading to high brightness. However, the quantum dot (QD)/ligand interaction also can modulate and control the interaction of the semiconductor core states with their environments. In many cases, producing functional nanocrystal systems necessitates an understanding of these chemical interactions as well as the ability to control what molecules are on the nanocrystal surface, their orientation, and binding geometry.

One overarching and motivating aspect of producing and exploring these various structures is to gain control over how charge and energy flow in systems designed to convert between various forms of energy within a variety of useful devices and architectures. Novel light emitting structures, electronic films, solids, and heterostructures, solar cells, photoelectrochemical electrodes, energy storage systems, thermoelectric devices, photocatalytic systems, and many other applications have been explored using these novel semiconductor nanostructures.

In this special issue, we have highlighted the broad and impressive research activities within the field of semiconductor nanocrystals. Researchers are pushing forward along many novel directions relevant to the fundamental photophysics of semiconductor

nanocrystals, developing a better understanding and control over the synthesis of nanocrystals, developing new semiconductor systems synthesized in the nanocrystal form, and the incorporation and utilization of the beneficial and tunable properties of the nanocrystals into various potential applications. The special issue has 51 contributions that span these areas of research. In the following, we group these research activities into eight research thrusts with 6–7 manuscripts per area. The manuscripts included in this special issue and these eight thrust areas are representative of the much broader research activities in the semiconductor QD community.

NEW SYNTHETIC METHODS

There are novel material or semiconductor systems where preparation methods of those systems into nanocrystals through solution phase chemistries are constantly being developed. In addition, new ways of synthesizing nanocrystals of the more common systems that achieve a higher monodispersity, better control of shape, larger batch yields, more reproducibility and stability, and larger range of ligand and surface chemistries are very active areas of research. Contributions in this research focus include the development of a novel ternary system HgInS and the further development of this family of semiconductors that include AgInS and CuInS by Stroyuk and co-workers,[1] the development of novel double (lead-free) metal–halide perovskite nanocrystals by Kshirsagar and Nag,[2] and the synthesis of $CsPbBr_3$ nanocrystals using a new phosphorous ligand to modify and improve their optical properties by McGrath and co-workers.[3] Finally, InP nanocrystals are of great commercial interest in light emitting applications, but the synthesis (especially of the larger systems with red emission wavelengths) and better control over size distribution are needed. Here, we have two contributions: one by McVey and co-workers exploring the use of Zn cations to improve surface passivation[4] and the other is a new core/shell structure from the work of Koh and co-workers that improves their stability.[5] In addition to novel synthetic methods, researchers continue to develop strategies to purify and refine the size-distribution of the as-synthesized structures. Wang and co-workers developed strategies to purify $CsPbX_3$ nanocrystals, which has been challenging due to their poor colloidal and structural stability.[6] Finally, Zhou and co-workers have developed novel synthesis of WS_2 platelets (a few monolayers) in nanoscale lateral dimensions and explored their carrier dynamics.[7]

NEW NANOSTRUCTURES

Building new types of nanostructures, including core/shell, giant core/shell, core shell/shell, and other types of heterostructures, is a very active area of nanocrystal research with many reports appearing monthly. In this special issue, we have a broad range of representative structures. Cassidy and Zamkov flipped the paradigm by making large core, thin shell particles.[8] The quantum confined states occur in the shell and not in the core. These types of structures control the optical and electronic properties in new and beneficial ways. Rafipoor and co-workers demonstrate that one needs to consider not only the lattice mismatch when building novel core/shell heterostructures but also the relative stiffness of the systems.[9] Abdu-Aguye and co-workers developed a novel Bi perovskite shell to improve PbS QDs processability, stability, and optical properties.[10] Drake and co-workers further developed their novel double heterostructure nanorod system with improved optical properties.[11] Panfil and co-workers developed the synthesis of quantum dot dimers of CdSe/CdS spherical nanostructures.[12] They demonstrated that the quantum confined states of the individual NCs couple when prepared as dimers. Finally, Dey and co-workers tethered CdSe nanocrystals to $CsPbBr_3$ nanoplatelets through organic ligands to induce novel functionality.[13]

CATION IMPURITY DOPING

Of particular interest in the nanocrystal community is the ability to perform controllable impurity doping of the nanostructures. Impurity dopants provide additional functionality. There are many different ways in which researchers have incorporated cation impurities into nanostructures, including low temperature cation exchange reactions. Here, we focus on impurity doping to induce novel functionality into the highly controlled nanostructures. Researchers are exploring impurity doping to induce electronic doping, magnetic functionality, and up- and down-conversion of photons. The contributions in this special issue span these efforts. Friedfeld and co-workers doped Zn^{2+} and Ga^{3+} into InP QDs; the incorporation of these dopant cations surprisingly improves their luminescent properties.[14] Kittilstved incorporated Fe^{3+} into ZnO nanocrystals and achieved air-stable *n*-type electronic doping, explored the simultaneous doping of Al and Fe, and detailed how these impurities modified the opto-electronic properties.[15] Fainblat and co-workers doped Co^{2+} into CdSe/CdS core/shell nanoplatelets to introduce additional magnetic–optical properties.[16] Yu and co-workers doped ZnSe with Mn^{2+} as a function of the nanocrystal shape and also explored ZnS and CdS doping.[17] Alam and co-workers replaced all the Pb^{2+} in $CsPbX_3$ nanocrystals with Eu^{2+}, producing a completely new material with novel functionality.[18] Finally, Parobek and co-workers provided an overview perspective on the use of Mn-doping to control hot electrons in nanocrystals for photocatalytic and other applications.[19]

SIZE DEPENDENT PROPERTIES

A hallmark of quantum-confined semiconductor nanocrystals is that they exhibit remarkable size-dependent properties. The most well studied and classic example is the emission wavelength. Despite 30 years of research, researchers continue to explore and discover new photoluminescence (PL) phenomena associated with the NC dimensions. In this special issue, there are several contributions of exploring the electronic structure and carrier dynamics as a function of the NC size and shape. Kasper and co-workers explored a size-dependent Rashba type spin–orbit coupling in ZnO NCs.[20] Sercel and co-workers developed a quasi-cubic model based on the effective mass approximation, including Rashba spin-orbits effects for metal–halide perovskite nanostructures.[21] Karpulevich and co-workers developed the size-dependent dielectric response function for colloidal nanocrystals.[22] The size-dependent absorption

cross section is an essential parameter needed for the study and utilization of semiconductor nanocrystals. Here, Puthenpurayil and co-workers determined the size-dependent absorption cross section for lead–halide perovskite nanocrystals.[23] The size- and temperature-dependent photoluminescence properties of methyl ammonium lead–halide perovskite nanocrystals were studied by Naghadeh and co-workers.[24] The absorption properties at low temperatures were studied as the function of the dimension in $CsPbI_3$ nanocrystals by Liu and co-workers.[25] Finally, since these colloidal semiconductor nanocrystals are ensemble systems, the size-dependent electrical and optical properties can be hidden by differing responses from nanocrystals of different sizes and shapes within the ensemble. Thus, studies at the single particle level can provide much needed insight, context, and understanding. Cao and co-workers studied two-photon excitation of single perovskite NCs through their PL emission.[26] The PL line shape is studied at the single QD level as a function of temperature by Podshivaylov and co-workers, and they elucidate the electron–phonon coupling in single CdSe nanocrystals.[27] Furthermore, most theories of NCs inherently assume a uniform spherical (or cuboid) shape, while the NCs actually are likely not these idealized structures. Here, Mcbride and Rosenthal provided an in-depth high-resolution electron microscopy study of quantum dot structures to elucidate their real structure.[28]

LIGAND/QD DYNAMICAL INTERACTIONS

Central to nanostructures are their surfaces and the organic molecules that decorate the surfaces. As a result, there are numerous studies regarding how ligands can have both positive and negative impact on the properties of nanostructures. The manuscripts here are a small representative sampling of this very active and vibrant area of nanoscience. Rigsby and co-workers studied how the triplet energy transfer from CdSe NCs surface bounds ligands depends upon the surface chemical binding in subtle ways.[29] They are developing strategies to use sensitized QD samples in triplet–triplet annihilation up-conversion schemes. The primary step is the triplet energy transfer from the NCs to the ligands. They studied here primary amines as the binding ligand and whether energy transfer occurs from core states or through trap states. Shang and co-workers investigated charge transfer from $CsPbI_3$ nanocrystal core states to surface bound dye molecules as a function of the NC size.[30] They used Marcus theory to explain both the charge transfer step and the back charge recombination step. The hole extraction was studied by Dutta and co-workers in CdSe QDs with nitroxide free radicals bound to their surfaces.[31] In contrast to many systems, they developed a strategy for hole extraction on ultrafast timescales. Hou and co-workers developed synthetic strategies to control the Auger recombination rate in CdSe based QDs.[32] Very efficient Auger recombination occurs in small sized NCs due to the spatial confinement of the carriers. This non-radiative recombination process limits the utility of NCs in many light emitting applications. Thus, developing strategies to reduce Auger recombination is a large effort within the nanocrystal community. Here, Peng demonstrates that by properly designing a heterostructure, the Auger rates can be reduced. Finally, Märker and co-workers made optically active ligands attach to CdSe QD surfaces and showed that they can utilize the optical properties of the QD and ligand for functional systems.[33] This work highlights a large research activity aiming to explore and control the beneficial properties of hybrid systems that incorporate organic and inorganic components to realize functionality that neither component could have in isolation.

LIGAND EFFECTS IN DIRECTING QD ASSEMBLIES

QD assemblies can display interesting properties distinct from those of isolated nanostructures. The ligands play a large role in directing the assembling of these nanocrystal/hybrid solids. Ligands can also modulate the opto-electronic properties of the resulting solids through defining the distance between the nanocrystals and inter-particle electronic interactions. Thus, controlling ligands for producing QD assemblies represents a large research effort in the nanocrystal community. Incorporating QDs in polymer blends can both stabilize and isolate the QDs, while conductive polymer/QD blends produce electronic access to the QD cores. Here, Mattoussi studied polymer stabilized QDs and Au structures through the lipoic acid group of the polymer.[34] The resulting colloids exhibited enhanced photostability. Strategies to prepare polymer linked colloidal gels were studied by Howard and co-workers through a thermodynamic computational study.[35] They mapped out the phase diagram of QD/linker gel formation as a function of the linker chains and developed design rules that could be used to realize various functionalities. Boron-doped Si nanocrystals produce nanocrystals where the boron dopants occupy surface sites and provide greater chemical flexibility. Greenhagen and co-workers developed strategies to utilize these boron sites to bind polyethylene glycol ligands and thereby allow for the Si nanocrystals to be stabilized in polar environments.[36] Nanostructured solids that incorporate nanostructures with DNA are fascinating systems. Most works in the literature study metal nanoparticle/DNA hybrid systems. Here, Dehankar and co-workers study DNA CdSe/CdS hybrid systems.[37] They developed strategies to bind the DNA to the QD surfaces and produced composites for detailed studies. Silva and co-workers studied the assembly of metal chalcogenide gels as a function of the reactivity that creates the assembly.[38] Different metal reactivity can lead to different functionality in the final solids. Since nanocrystals are typically not the idealized spheres that are typically envisioned but rather highly faceted, they can be assembled into structures that are not close packed, depending on the facet/ligand interactions and facet/facet interactions between neighboring nanocrystals. Soligno and Vanmaekelbergh have utilized these features to assemble novel 2D QD arrays with various patterns. Here, they developed design rules for assembling these structures.[39] Winslow and co-workers developed strategies based upon neutron scattering measurements to elucidate the QD/ligand structure.[40]

QD FUNCTIONAL SOLIDS AND DEVICES

QDs are being incorporated into various functional solids and devices. For about ten years, PbS, CdSe, and $CsPbI_3$ QDs have been incorporated and investigated in QD based solar cells, where the QDs are the photoactive species. Typically, they are incorporated into solution-deposited thin films, but sometimes, polymer/QD bulk

heterojunctions are also studied. The certified power conversion efficiency (PCE) of QD solar cells has steadily increased from ~3% to over 15% as a result of a very active research community. Such progress has provided ample encouragement to the research community to continue working in these areas. Here, Lin and co-workers simulated the IV characteristics of PbS based QD solar cells in order to provide design rules for further improving the PCE of these systems and devices.[41] Greaney and co-workers studied solar cells fabricated from CdSe in P3HT as a bulk heterojunction solar cell[42] and determined how the nanocrystalC surface chemistry impacts the final device performance and thus provided guidelines for developing the next generation of QD/polymer bulk heterojunctions. QDs are interesting for solar energy conversion because they possess unique advantages that can go beyond traditional bulk and thin film systems. Califano *et al.* tackled the concept of an intermediate-band solar cell with quantum dots as the active component.[43] The intermediate band concept can surpass single junction efficiency limits and thus necessitates continued research activity. The flip side to the photovoltaic concept is photodetectors. QDs have numerous advantages in this area especially for infrared detectors. Guyot-Sionnest and co-workers provided a perspective on QDs for infrared photodetectors and detailed why QDs are useful for this application.[44] Ahn and co-workers demonstrated that fabricating hybrids of PbS QDs and graphene can increase the photoresponse of the QDs.[45] Transparent conductors can potentially also benefit from heavily doped wide bandgap semiconductor nanocrystals as the colloidal systems offer processing advantages. Here, Gudjonsdottir and co-workers studied electrochemically doped ZnO QDs.[46] Finally, Westmoreland and co-workers provided a perspective on incorporating and coupling QDs with plasmons and into optical microcavities.[47] QD dots have unique advantages for such systems, and these could be developed for photocatalytic and light emitting applications.

QDS IN PHOTOCATALYTIC APPLICATIONS

One of the first applications targeted by semiconductor nanocrystals was for photocatalysis. The size-dependent band edges that govern the size-dependent light emission imply a size-dependent reduction/oxidation potential. Thus, there are ongoing studies utilizing and incorporating semiconductor nanocrystals into various photocatalytic applications. Here, Yin and co-workers explored CdTe quantum dots for photogenerated hydrogen.[48] They find that there is an optimal size for hydrogen generation: too big and the generation efficiency suffers, and too small and the QDs are not photostable. Hu and co-workers detailed studies using $CuInS_2$/ZnS core/shell quantum dots for hydrogen generation.[49] They studied the Cu-to-In ratio in the nanocrystals and found that Cu-deficient nanocrystals performed better. Chauhan and co-workers are also interested in photocatalytic hydrogen generation. They studied a heterostructure between V_2O_5 and CdX systems.[50] This new class of heterostructures is type II and promotes beneficial charge separation in order to drive photoredox reactions. Finally, Lu and co-workers demonstrated that the ligand identity can also tune the band edges (redox potentials) for driving different types of photoinduced carbon–carbon bond forming reactions.[51]

CONCLUSION

The field of semiconductor nanocrystals, as represented by the articles in this special issue, is a vibrant and active research community, with steep progress in an every-growing set of subfields. Despite more than 30 years of research, new structures are constantly being developed, and novel synthetic strategies that improve upon traditional methods are constantly being reported. Incorporating these novel structures into functional systems for a variety of applications is ongoing. There are many small and large companies that are marketing and developing a few of these applications. Quantum dot-based displays are available for purchase. We expect that these trends will continue and are very excited about the future prospects of semiconductor nanocrystal systems.

ACKNOWLEDGMENTS

We thank all of the authors who contributed to this special issue. The quality of the published manuscripts and the number of submissions all point to a very vibrant and growing community with novel insights and new advances to come. We also want to thank the editorial staff at the Journal of Chemical Physics for their help and support for this special issue.

REFERENCES

[1]O. Stroyuk, A. Raevskaya, F. Spranger, O. Selyshchev, V. Dzhagan, D. Solonenko, N. Gaponik, D. R. T. Zahn, and A. Eychmüller, "Mercury-indium-sulfide nanocrystals: A new member of the family of ternary in based chalcogenides," J. Chem. Phys. **151**, 144701 (2019).

[2]A. S. Kshirsagar and A. Nag, "Synthesis and optical properties of colloidal $Cs_2AgAb_{1-X}Bi_xCl_6$ double perovskite nanocrystals," J. Chem. Phys. **151**, 161101 (2019).

[3]F. McGrath, U. V. Ghorpade, and K. M. Ryan, "Synthesis and dimensional control of $CsPbBr_3$ perovskite nanocrystals using phosphorous based ligands," J. Chem. Phys. **152**, 174702 (2020).

[4]B. F. P. McVey, R. A. Swain, D. Lagarde, Y. Tison, H. Martinez, B. Chaudret, C. Nayral, and F. Delpech, "Unraveling the role of zinc complexes on indium phosphide nanocrystal chemistry," J. Chem. Phys. **151**, 191102 (2019).

[5]S. Koh, H. Lee, T. Lee, K. Park, W.-J. Kim, and D. C. Lee, "Enhanced thermal stability of InP quantum dots coated with Al-doped ZnS shell," J. Chem. Phys. **151**, 144704 (2019).

[6]C. Wang, A. S. R. Chesman, W. Yin, L. Frazer, A. M. Funston, and J. J. Jasieniak, "Facile purification of $CsPbX_3$ ($X = Cl^-, Br^-, I^-$) perovskite nanocrystals," J. Chem. Phys. **151**, 121105 (2019).

[7]P. Zhou, I. Tanghe, P. Schiettecatte, D. van Thourhout, Z. Hens, and P. Geiregat, "Ultrafast carrier dynamics in colloidal WS_2 nanosheets obtained through a hot injection synthesis," J. Chem. Phys. **151**, 164701 (2019).

[8]J. Cassidy and M. Zamkov, "Nanoshell quantum dots: Quantum confinement beyond the exciton Bohr radius," J. Chem. Phys. **152**, 110902 (2020).

[9]M. Rafipoor, H. Tornatzky, D. Dupont, J. Maultzsch, M. D. Tessier, Z. Hens, and H. Lange, "Strain in InP/ZnSe, S core/shell quantum dots from lattice mismatch and shell thickness—Material stiffness influence," J. Chem. Phys. **151**, 154704 (2019).

[10]M. Abdu-Aguye, D. Bederak, S. Kahmann, N. Killilea, M. Sytnyk, W. Heiss, and M. A. Loi, "Photophysical and electronic properties of bismuth-perovskite shelled lead sulfide quantum dots," J. Chem. Phys. **151**, 214702 (2019).

[11]G. A. Drake, J. C. Flanagan, and M. Shim, "Highly luminescent double-heterojunction nanorods," J. Chem. Phys. **151**, 134706 (2019).

[12]Y. E. Panfil, D. Shamalia, J. Cui, S. Koley, and U. Banin, "Electronic coupling in colloidal quantum dot molecules; the case of CdSe/CdS core/shell homodimers," J. Chem. Phys. **151**, 224501 (2019).

[13]S. Dey, H. Cohen, I. Pinkas, H. Lin, M. Kazes, and D. Oron, "Band alignment and charge transfer in $CsPbBr_3$–CdSe nanoplatelet hybrids coupled by molecular linkers," J. Chem. Phys. **151**, 174704 (2019).
[14]M. R. Friedfeld, J. L. Stein, D. A. Johnson, N. Park, N. A. Henry, M. J. Enright, D. Mocatta, and B. M. Cossairt, "Effects of Zn^{2+} and Ga^{3+} doping on the quantum yield of cluster-derived InP quantum dots," J. Chem. Phys. **151**, 194702 (2019).
[15]E. Buz, D. Zhou, and K. R. Kittilstved, "Air-stable n-type Fe-doped ZnO colloidal nanocrystals," J. Chem. Phys. **151**, 134702 (2019).
[16]R. Fainblat, S. Delikanli, L. Spee, T. Czerny, F. Isik, V. K. Sharma, H. V. Demir, and G. Bacher, "Impurity incorporation and exchange interactions in Co^{2+}-doped CdSe/CdS core/shell nanoplatelets," J. Chem. Phys. **151**, 224708 (2019).
[17]J. H. Yu, J. Kim, T. Hyeon, and J. Yang, "Facile synthesis of manganese (II)-Doped ZnSe nanocrystals with controlled dimensionality," J. Chem. Phys. **151**, 244701 (2019).
[18]F. Alam, K. D. Wegner, S. Pouget, L. Amidani, K. Kvashnina, D. Aldakov, and P. Reiss, "Eu^{2+}: A suitable substituent for Pb^{2+} in $CsPbX_3$ perovskite nanocrystals?," J. Chem. Phys. **151**, 231101 (2019).
[19]D. Parobek, T. Qiao, and D. H. Son, "Energetic hot electrons from exciton-to-hot electron upconversion in Mn-doped semiconductor nanocrystals," J. Chem. Phys. **151**, 120901 (2019).
[20]J. M. Kasper, D. R. Gamelin, and X. Li, "Theoretical investigation of quantum confinement on the Rashba effect in ZnO semiconductor nanocrystals," J. Chem. Phys. **152**, 014308 (2020).
[21]P. C. Sercel, J. L. Lyons, N. Bernstein, and A. L. Efros, "Quasicubic model for metal halide perovskite nanocrystals," J. Chem. Phys. **151**, 234106 (2019).
[22]A. Karpulevich, H. Bui, Z. Wang, S. Hapke, C. Palencia Ramírez, H. Weller, and G. Bester, "Dielectric response function for colloidal semiconductor quantum dots," J. Chem. Phys. **151**, 224103 (2019).
[23]J. Puthenpurayil, O. H.-C. Cheng, T. Qiao, D. Rossi, and D. H. Son, "On the determination of absorption cross section of colloidal lead halide perovskite quantum dots," J. Chem. Phys. **151**, 154706 (2019).
[24]S. B. Naghadeh, S. Sarang, A. Brewer, A. L. Allen, Y.-H. Chiu, Y.-J. Hsu, J.-Y. Wu, S. Ghosh, and J. Z. Zhang, "Size and temperature dependence of photoluminescence of hybrid perovskite nanocrystals," J. Chem. Phys. **151**, 154705 (2019).
[25]A. Liu, L. G. Bonato, F. Sessa, D. B. Almeida, E. Isele, G. Nagamine, L. F. Zagonel, A. F. Nogueira, L. A. Padilha, and S. T. Cundiff, "Effect of dimensionality on the optical absorption properties of $CsPbI_3$ perovskite nanocrystals," J. Chem. Phys. **151**, 191103 (2019).
[26]Z. Cao, B. Lv, H. Zhang, Y. Lv, C. Zhang, Y. Zhou, X. Wang, and M. Xiao, "Two-photon excited photoluminescence of single perovskite nanocrystals," J. Chem. Phys. **151**, 154201 (2019).
[27]E. A. Podshivaylov, M. A. Kniazeva, A. A. Gorshelev, I. Y. Eremchev, A. V. Naumov, and P. A. Frantsuzov, "Contribution of electron-phonon coupling to the luminescence spectra of single colloidal quantum dots," J. Chem. Phys. **151**, 174710 (2019).
[28]J. R. McBride and S. J. Rosenthal, "Real colloidal quantum dot structures revealed by high resolution analytical electron microscopy," J. Chem. Phys. **151**, 160903 (2019).
[29]E. M. Rigsby, K. Lee, J. Sun, D. A. Fishman, and M. L. Tang, "Primary amines enhance triplet energy transfer from both the band edge and trap state from CdSe nanocrystals," J. Chem. Phys. **151**, 174701 (2019).
[30]Q. Shang, A. L. Kaledin, Q. Li, and T. Lian, "Size dependent charge separation and recombination in $CsPbI_3$ perovskite quantum dots," J. Chem. Phys. **151**, 074705 (2019).
[31]P. Dutta, Y. Tang, C. Mi, M. Saniepay, J. A. McGuire, and R. Beaulac, "Ultrafast hole extraction from photoexcited colloidal CdSe quantum dots coupled to nitroxide free radicals," J. Chem. Phys. **151**, 174706 (2019).
[32]X. Hou, Y. Li, H. Qin, and X. Peng, "Effects of interface-potential smoothness and wavefunction delocalization on auger recombination in colloidal CdSe-based core/shell quantum dots," J. Chem. Phys. **151**, 234703 (2019).
[33]B. Märker, J. Hiller, F. Wackenhut, K. Braun, A. Meixner, and M. Scheele, "Simultaneous positive and negative optical patterning with dye-sensitized CdSe quantum dots," J. Chem. Phys. **151**, 141102 (2019).
[34]Z. Jin, A. Kapur, W. Wang, J. Diaz Hernandez, M. Thakur, and H. Mattoussi, "The dual–function of lipoic acid groups as surface anchors and sulfhydryl reactive sites on polymer–stabilized QDs and Au nanocolloids," J. Chem. Phys. **151**, 164703 (2019).
[35]M. P. Howard, R. B. Jadrich, B. A. Lindquist, F. Khabaz, R. T. Bonnecaze, D. J. Milliron, and T. M. Truskett, "Structure and phase behavior of polymer-linked colloidal gels," J. Chem. Phys. **151**, 124901 (2019).
[36]J. R. Greenhagen, H. P. Andaraarachchi, Z. Li, and U. R. Kortshagen, "Synthesis of PEG-grafted boron doped Si nanocrystals," J. Chem. Phys. **151**, 211103 (2019).
[37]A. Dehankar, T. Porter, J. A. Johnson, C. E. Castro, and J. O. Winter, "Compact quantum dot surface modification to enable emergent behaviors in quantum dot-DNA composites," J. Chem. Phys. **151**, 144706 (2019).
[38]K. L. Silva, L. Silmi, and S. L. Brock, "Effect of metal ion solubility on the oxidative assembly of metal sulfide quantum dots," J. Chem. Phys. **151**, 234715 (2019).
[39]G. Soligno and D. Vanmaekelbergh, "Phase diagrams of honeycomb and square nanocrystal superlattices from the nanocrystal's surface chemistry at the dispersion-air interface," J. Chem. Phys. **151**, 234702 (2019).
[40]S. W. Winslow, W. Shcherbakov-Wu, Y. Liu, W. A. Tisdale, and J. W. Swan, "Characterization of colloidal nanocrystal surface structure using small angle neutron scattering and efficient Bayesian parameter estimation," J. Chem. Phys. **150**, 244702 (2019).
[41]W. M. M. Lin, N. Yazdani, O. Yarema, S. Volk, M. Yarema, T. Kirchartz, and V. Wood, "Simulating nanocrystal-based solar cells: A lead sulfide case study," J. Chem. Phys. **151**, 241104 (2019).
[42]M. J. Greaney, J. Joy, B. A. Combs, S. Das, J. J. Buckley, S. E. Bradforth, and R. L. Brutchey, "Effects of interfacial ligand type on hybrid P3HT:CdSe quantum dot solar cell device parameters," J. Chem. Phys. **151**, 074704 (2019).
[43]M. Califano, E. S. Skibinsky-Gitlin, F. M. Gómez-Campos, and S. Rodríguez-Bolívar, "New strategies for colloidal-quantum-dot-based intermediate-band solar cells," J. Chem. Phys. **151**, 154101 (2019).
[44]P. Guyot-Sionnest, M. M. Ackerman, and X. Tang, "Colloidal quantum dots for infrared detection beyond silicon," J. Chem. Phys. **151**, 060901 (2019).
[45]S. Ahn, H. Chung, W. Chen, M. A. Moreno-Gonzalez, and O. Vazquez-Mena, "Optoelectronic response of hybrid PbS-QD/Graphene photodetectors," J. Chem. Phys. **151**, 234705 (2019).
[46]S. Gudjonsdottir, C. Koopman, and A. J. Houtepen, "Enhancing the stability of the electron density in electrochemically doped ZnO quantum dots," J. Chem. Phys. **151**, 144708 (2019).
[47]D. E. Westmoreland, K. P. McClelland, K. A. Perez, J. C. Schwabacher, Z. Zhang, and E. A. Weiss, "Properties of quantum dots coupled to plasmons and optical cavities," J. Chem. Phys. **151**, 210901 (2019).
[48]J. Yin, N. M. B. Cogan, R. Burke, Z. Hou, K. L. Sowers, and T. D. Krauss, "Size dependence of photocatalytic hydrogen generation for CdTe quantum dots," J. Chem. Phys. **151**, 174707 (2019).
[49]W. Hu, S. Yang, and J. Huang, "Composition effect on the carrier dynamics and catalytic performance of $CuInS_2$/ZnS quantum dots for light driven hydrogen generation," J. Chem. Phys. **151**, 214705 (2019).
[50]S. Chauhan, A. Sheng, J. Cho, S. A. Razek, N. Suwandaratne, M. Y. Sfeir, L. F. J. Piper, S. Banerjee, and D. F. Watson, "Type-II heterostructures of α-V_2O_5 nanowires interfaced with cadmium chalcogenide quantum dots: Programmable energetic offsets, ultrafast charge transfer, and photocatalytic hydrogen evolution," J. Chem. Phys. **151**, 224702 (2019).
[51]H. Lu, X. Zhu, C. Miller, J. San Martin, X. Chen, E. M. Miller, Y. Yan, and M. C. Beard, "Enhanced photoredox activity of $CsPbBr_3$ nanocrystals by quantitative colloidal ligand exchange," J. Chem. Phys. **151**, 204305 (2019).