Multi-excitons and correlation effects in perovskite nanocrystals

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Up to date, perovskites have remained to be one of the most fashionable names in the research of photovoltaic materials, achieving an efficiency reaching over 25% without the use of tandem structure [1]. Apart from being excellent materials for solar cells, perovskites have also shown to be an extremely promising candidate for both classical and quantum light sources [2, 3]. Recent advancements in synthesis and surface treatment have allowed a more precise control of emission from nanostructures [4, 5]. In this context, our theoretical work aims to investigate the electronic and optical properties of the systems of single exciton and beyond. Previous calculations on nanocubes or spherical nanocrystals have demonstrated the correlation origin of exciton fine-structure [6] and biexciton/trion emission [7]. In this talk, we will present the configuration interaction approach to take into account the correlation effects in these systems in a more systematic and complete manner.

REFERENCES

[1] Kim et al., High-Efficiency Perovskite Solar Cells, Chem. Rev. 2020, 120, 7867-7918, 2020
[2] Protesescu et al., Nanocrystals of cesium lead halide perovskites (cspbx3, x = cl, br, and i): Novel optoelectronic materials showing bright emission with wide color gamut. Nano Letters, 15(6):3692–3696, 2015
[3] Utzat et al., Coherent single-photon emission from colloidal lead halide perovskite quantum dots. Science, 363(6431):1068–1072, 2019
[4] Huo et al., Optical Spectroscopy of Single Colloidal CsPbBr3 Perovskite Nanoplatelets, Nano Lett. 2020, 20, 5, 3673–3680
[5] Bertolloti et al., Crystal Structure, Morphology, and Surface Termination of Cyan-Emissive, Six-Monolayers-Thick CsPbBr3 Nanoplatelets from X-ray Total Scattering, ACS Nano 2019, 13, 12, 14294–14307
[6] Tamarat et al., The dark exciton ground state promotes photon-pair emission in individual perovskite nanocrystals, Nature Communications, vol 11, 6001, 2020
[7] Nguyen et al., Calculation of the biexciton shift in nanocrystals of inorganic perovskites. Phys. Rev. B, 101. 125424, 2020

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