

MAS17-2017-000066

Abstract for an Invited Paper
for the MAS17 Meeting of
the American Physical Society

Electronic and Optical Properties of Lead Halide Perovskite Nanocrystals

ALEXANDER EFROS, Naval Research Lab

The growing attention to perovskite nanocrystals is connected with their unusual and potentially useful electronic and optical properties. I will discuss the bulk energy band structure of CsPbX_3 ($X = \text{I}, \text{Cl}, \text{and Br}$) perovskites and show that all of them have the band edge at R-point of the Brillouin zone. To describe electronic and optical properties of perovskite nanocrystals we have derived the four band effective mass Hamiltonian, which describes the electronic properties of electron and holes near the band edge. Using this Hamiltonian we calculate the lowest quantum confined levels of electrons and holes and the spectra of the allowed optical transitions. The calculations takes into account the cubic shape of the perovskite nanocrystals, that results into inhomogeneous electric field of emitted and absorb photons. The symmetry of the ground exciton state has been analyzed and the radiative decay time has been calculated. The results of our theoretical calculations are in a good agreement with available experimental data.