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Anomalous Suppression of Valley Splittings in Lead Salt Nanocrystals ALEXANDER PODDUBNY, MIKHAIL NESTOKLON, Ioffe Institute, Russian Academy of Sciences, SERGUEI GOUPALOV¹, Jackson State University — Atomistic $sp^3d^5s^*$ tight-binding theory of PbSe and PbS nanocrystals is developed. It is demonstrated, that the valley splittings of confined electrons and holes strongly and peculiarly depend on the geometry of a nanocrystal. When the nanocrystal lacks a microscopic center of inversion and has T_d symmetry, the splittings are strongly suppressed as compared to the more symmetric nanocrystals with O_h symmetry, having an inversion center. This effect is quite unusual because typically a higher symmetry of a physical system implies a higher degeneracy of its energy levels, while in our case the suppression of the splittings occurs in NCs having lower symmetry. Nevertheless, we were able to explain this puzzling behavior using mathematical apparatus of the group theory.

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