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Elimination of deep surface traps in charged colloidal PbS and CdSe quantum dots OLEKSANDR VOZNYY, SUSANNA THON, ALEX IP, EDWARD SARGENT, University of Toronto — Colloidal quantum dots (CQDs) offer a promising path towards high efficiency, scalable, solution and room processed photovoltaics and electronics. Their promise is curtailed today by difficulty of doping, inefficient transport, nonradiative recombination, and blinking, all generally attributed to electronic trap formation. Using first-principles simulations on off-stoichiometric colloidal quantum dots, we show that preparing a CQD free of traps is possible. However, self-compensating defects can form deep electronic trap states in response to charging or doping even in the most idealized CQDs. Surface traps arise from atomic dimers whose energy levels reside within the bandgap. The same states can also form upon photoexcitation, providing an atomistic mechanism for blinking. We show that avoiding the trap formation upon doping is possible by incorporation of select cations on the surface which shift the dimer energy levels above the quantum-confined bandedge.

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