

Abstract Submitted  
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**Numerical Study of Carrier Multiplication in Nanocrystalline form of PbSe and PbS and the bulk** ANDREI PIRYATINSKI, KIRILL VELIZHANIN, Theoretical Division, Los Alamos National Lab — Using previously developed Exciton Scattering Model, we report on systematic numerical study of the carrier multiplication (CM) dynamics in spherically symmetric PbSe and PbS nanocrystals (NCs) and bulk. The quantum efficiency (QE) associated with the photogeneration and population relaxation processes are calculated. It is found that the photogeneration event provides small, about 5%, contribution to the total QE compared to the contribution from the population relaxation process. The analysis shows that the impact ionization dynamics is the main mechanism responsible for the CM during *both* the photogeneration and the population relaxation events. Furthermore, the calculated photogeneration and total QEs for various size NCs are found never to exceed the calculated limiting values for bulk. This observation is explained in terms of the quantum-confinement induced weak effective Coulomb enhancement whose contribution to the impact ionization rate is fully suppressed by the reduction in the biexciton density of states. We also find weak dependence of the total QE on the transform limited pump pulse duration. Comparison of the calculated QEs to published experimental data shows that our calculations well reproduce the experimentally observed trends.

Andrei Piryatinski  
Theoretical Division, Los Alamos National Lab

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