Experiments and computational modeling of exciton formation, nonlinear quenching, and radiative emission at high excitation density and strong spatial gradients -- e.g. particle track and laser focus

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Our goal is to develop and validate a computational model of proportionality between luminescence light yield in the track of a high energy electron and the initial energy of the primary electron based on material parameters such as rate constants and transport coefficients. We report both the model, with significant expansion of included physics from the version that we reported in 2011[1], and the measurement of some of the necessary material parameters[2,3] for input. The model is based on a system of diffusion-limited coupled rate equations describing electron, hole, and exciton transport and mutual interaction in the pure host, plus 3 additional equations for each activator or co-dopant added to the host. The equations are solved by a finite element method for assumed cylindrical track geometry. The expanded model includes hot electron diffusion enabling treatment of charge separation in halides, as well as slower processes of carrier trapping and release during the subsequent electric-field driven recombination. Picosecond optical absorption allows determination of rate constants for carrier capture on activators and electron capture on self-trapped holes[2]. Interband z-scan experiments provide 2nd and 3rd order rate constants of nonlinear quenching[3]. We solve the rate and transport equations in the geometry of idealized electron tracks, subject to linear energy deposition dE/dx simulated with the Geant4 Monte Carlo code. The predictions of proportionality and light yield are compared to Compton-coincidence measurements and gamma yield spectra. For the first time, a consistent account of the quite different proportionality curves for undoped CsI at 295 K and 100 K and CsI:Tl at 295 K is obtained on this basis.

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Note received: Please find in the upload my abstract submitted for oral presentation at EXCON 2015 in the Session Ultrafast dynamics of excitons; relaxation, energy transport, charge transfer. Xinfu Lu is listed as first author. R. T. Williams is the speaker and corresponding author.