Supplementary Material

Impact of doping on InAs/GaAs quantum-dot solar cells: a numerical study on photovoltaic and photoluminescence behavior

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- Figure S1: Optical absorption data.
- Figures S2-S6: Synoptic figures summarizing the results of the numerical simulation of the solar cells discussed in the manuscript, namely:
  - Reference bulk cell, Fig. S2
  - Undoped QD cell, Fig. S3
  - Modulation doped QD cell, with $\alpha = 4$ e/dot, Fig. S4
  - Directly doped QD cell, with $\alpha = 18$ e/dot, Fig. S5
  - Uniformly doped QD cell, with $\alpha = 8$ e/dot, Fig. S6.

  SRH lifetime is set to 10 ns. For each doping strategy, the doping levels are those corresponding to the maximum achievable cell efficiency.
- Figure S7: Integrated PhotoLuminescence at open circuit condition for the various doping methods.

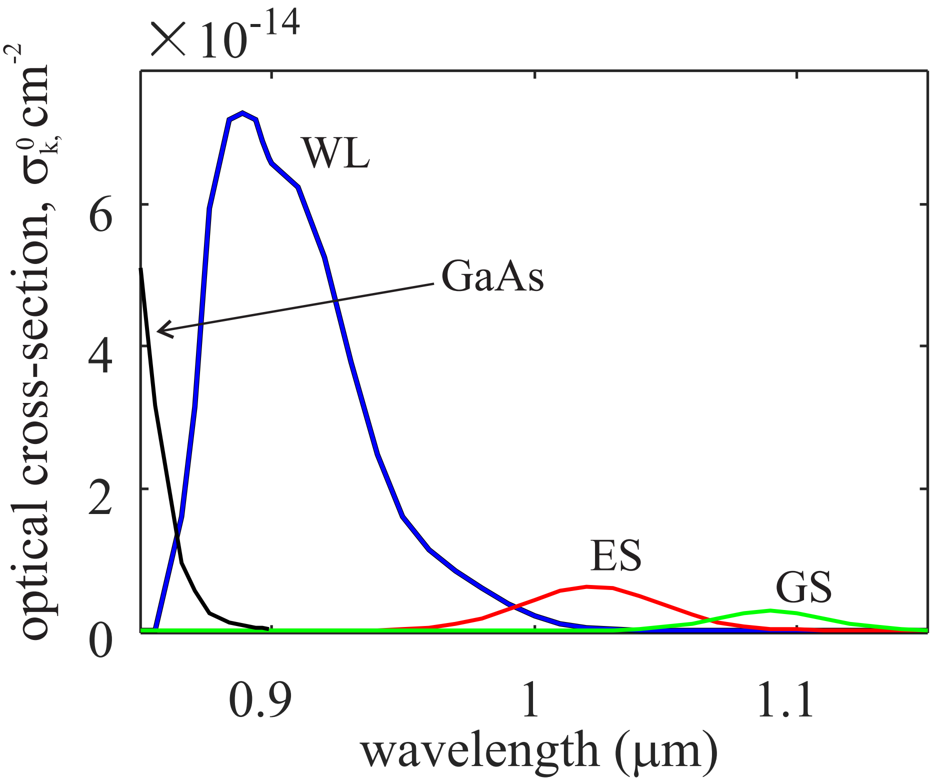

Figure S1: Wavelength dependence of the optical cross-section, σ_k^0, relative to the WL, ES and GS states used in the simulations (solid lines). The corresponding optical absorption coefficient can be evaluated as $\alpha_{\mathrm{k}}^0 = \sigma_{\mathrm{k}}^0 N_{\mathrm{QD}}/t_{\mathrm{QD}}$, N_{QD} and t_{QD} being the QD areal density and thickness, respectively. For the sake of reference also the bulk optical absorption tail is quoted.

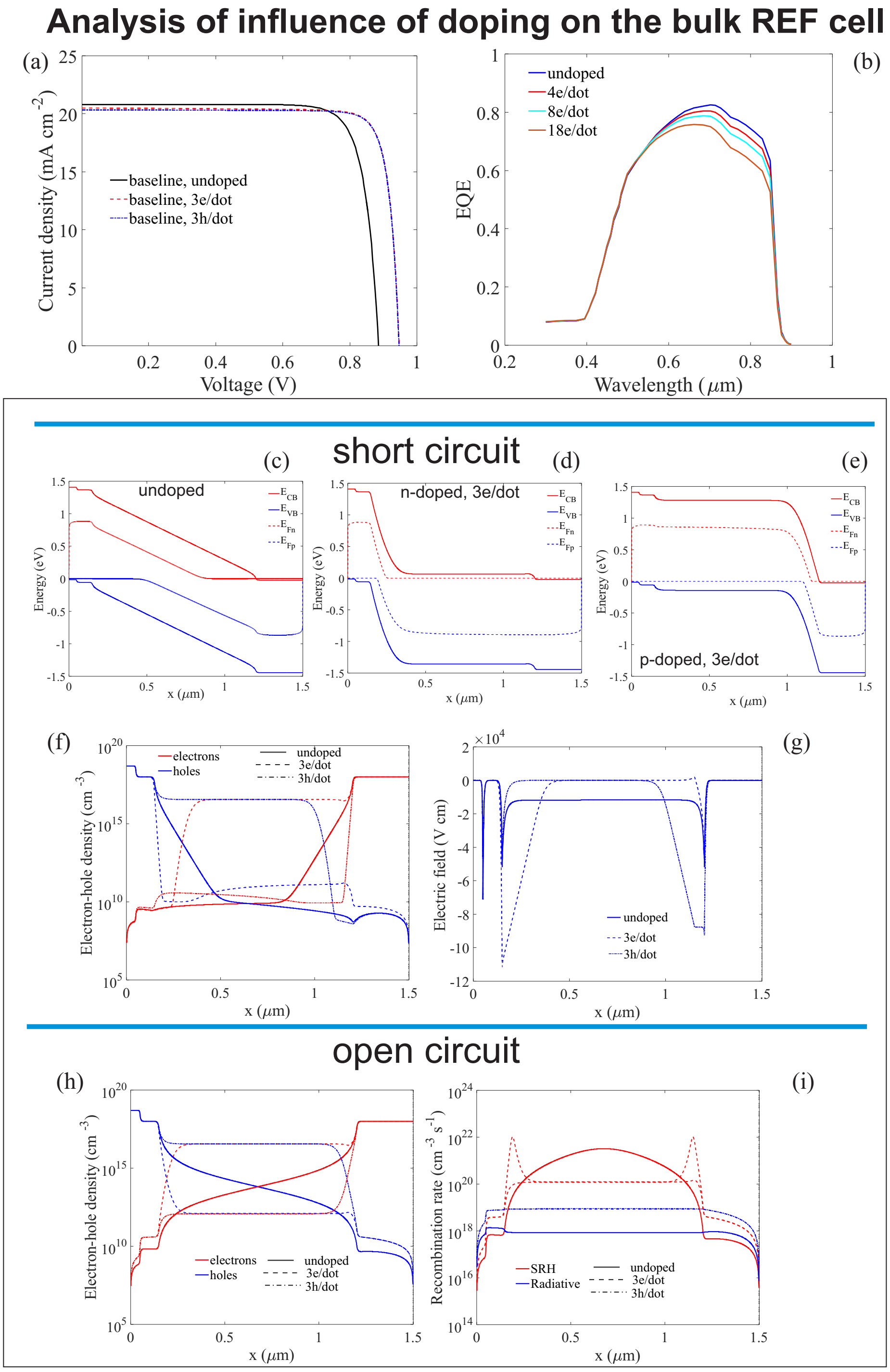

Figure S2: (a) *J*-*V* for undoped, *n*-doped and *p*-doped base. The quoted 3 e(h)/dot doping density means a uniform doping level of 3.6×10^{16} cm^{-3}; (b) EQE for different levels of *n*-type doping. (c)-(e) Band diagram at short circuit for the undoped, *n*-doped and *p*-doped base. (f) Free carriers density and (g) electric field profile at short circuit. (h) Free carriers density and (i) recombination rates distribution at open circuit condition.

undoped cell

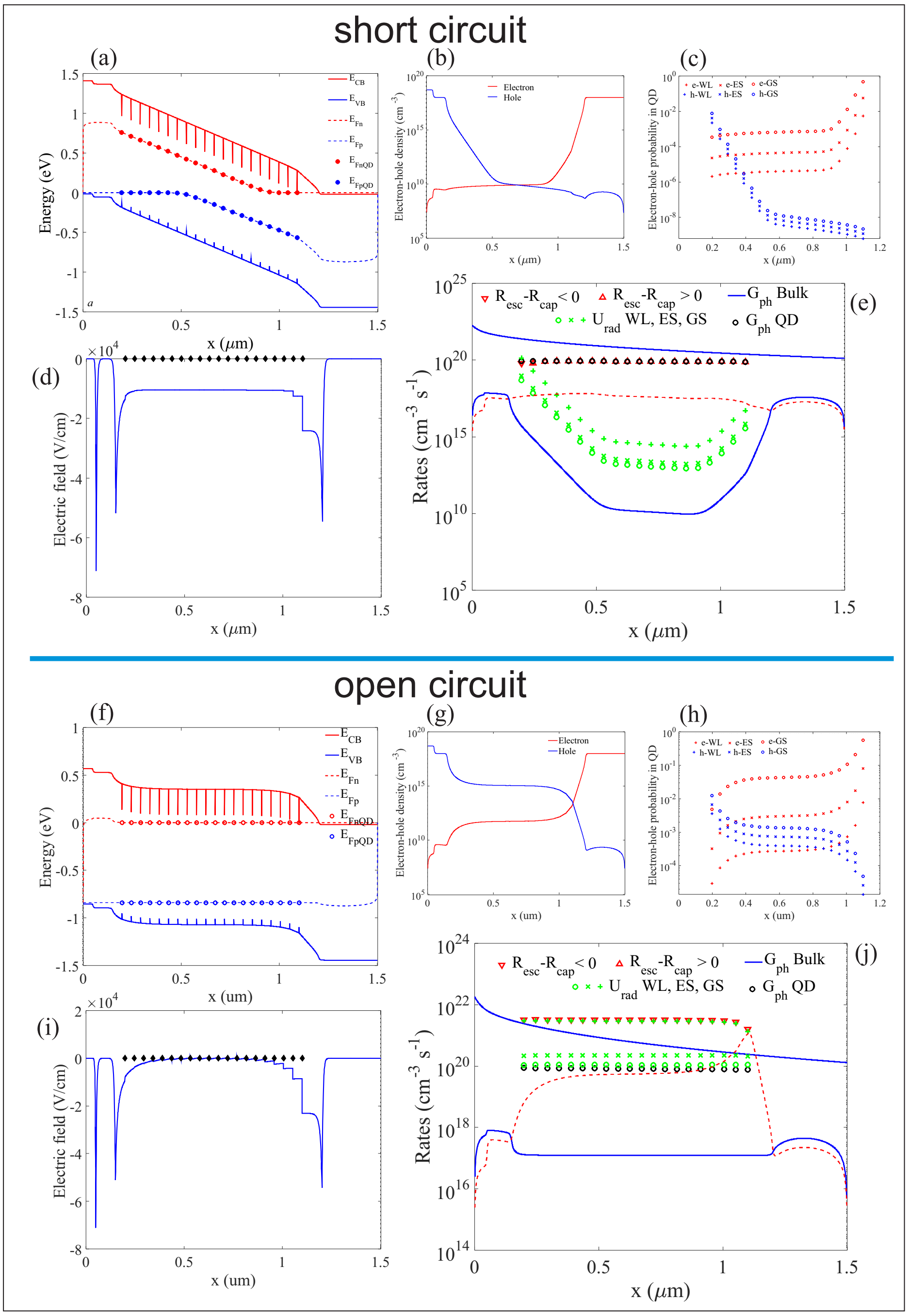

Figure S3: Spatial distribution at short circuit condition of energy bands (a), free carriers density (b), QD occupation probability (c), electric field (d), recombination rates (e). Spatial distribution at open circuit condition of energy bands (f), free carriers density (g), QD occupation probability (h), electric field (i), recombination rates (j). Diamond symbols in the electric field figures (d) and (i) indicate the QD layers position.

modulation doped cell, 4e/dot

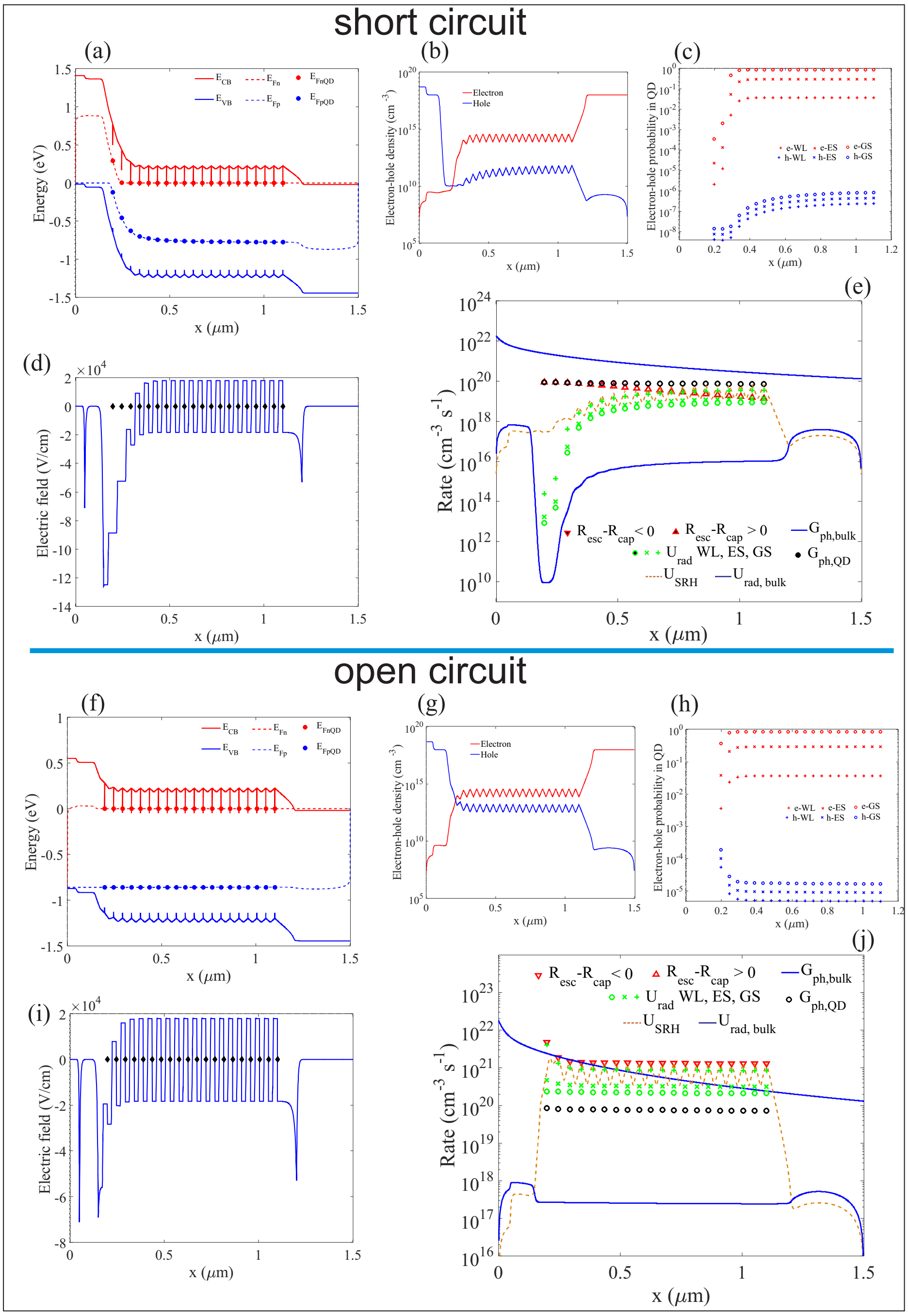

Figure S4: Spatial distribution at short circuit condition of energy bands (a), free carriers density (b), QD occupation probability (c), electric field (d), recombination rates (e). Spatial distribution at open circuit condition of energy bands (f), free carriers density (g), QD occupation probability (h), electric field (i), recombination rates (j). Diamond symbols in the electric field figures (d) and (i) indicate the QD layers position.

direct doped cell, 18e/dot

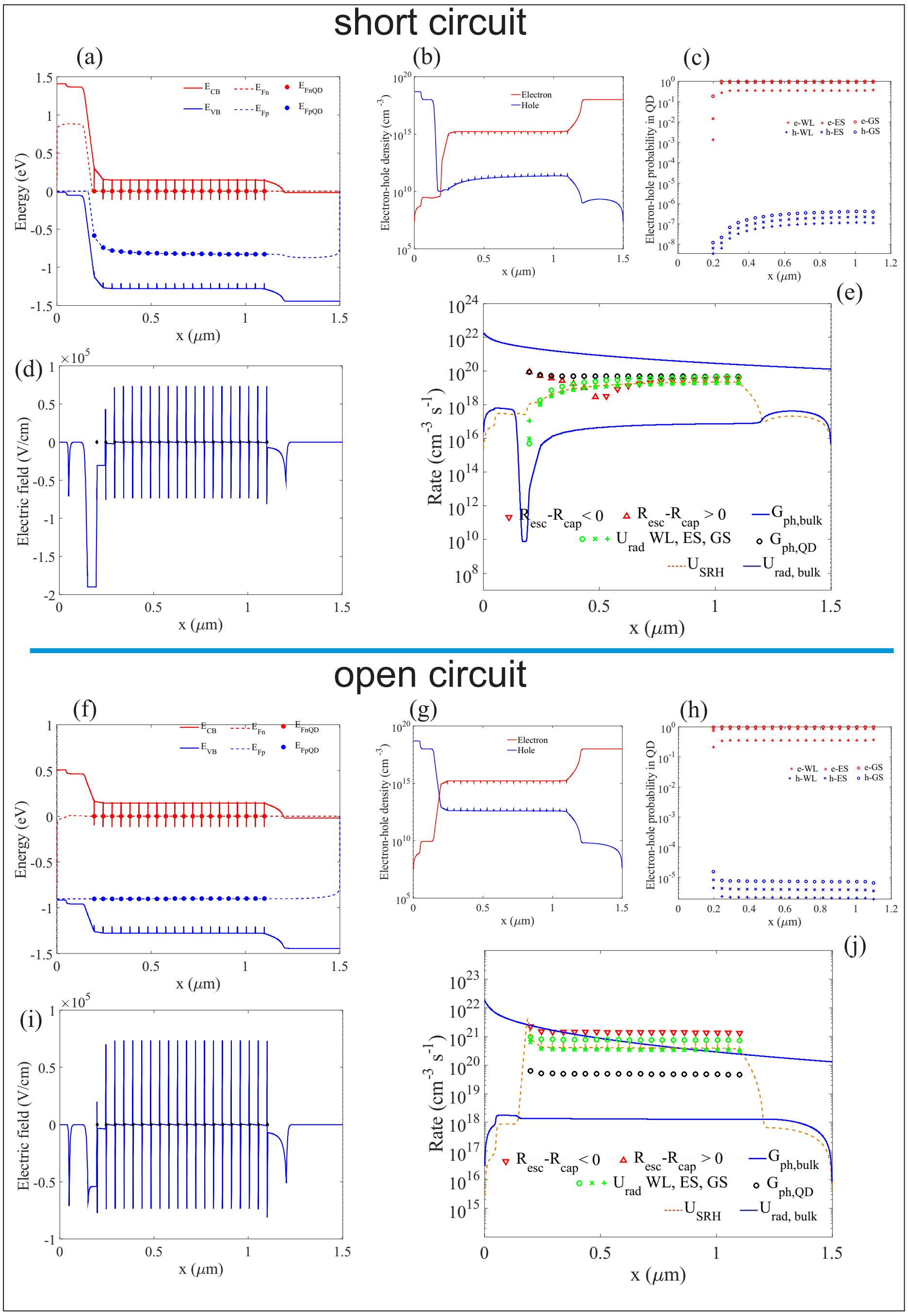

Figure S5: Spatial distribution at short circuit condition of energy bands (a), free carriers density (b), QD occupation probability (c), electric field (d), recombination rates (e). Spatial distribution at open circuit condition of energy bands (f), free carriers density (g), QD occupation probability (h), electric field (i), recombination rates (j). Diamond symbols in the electric field figures (d) and (i) indicate the QD layers position.

uniformly doped cell, 8e/dot

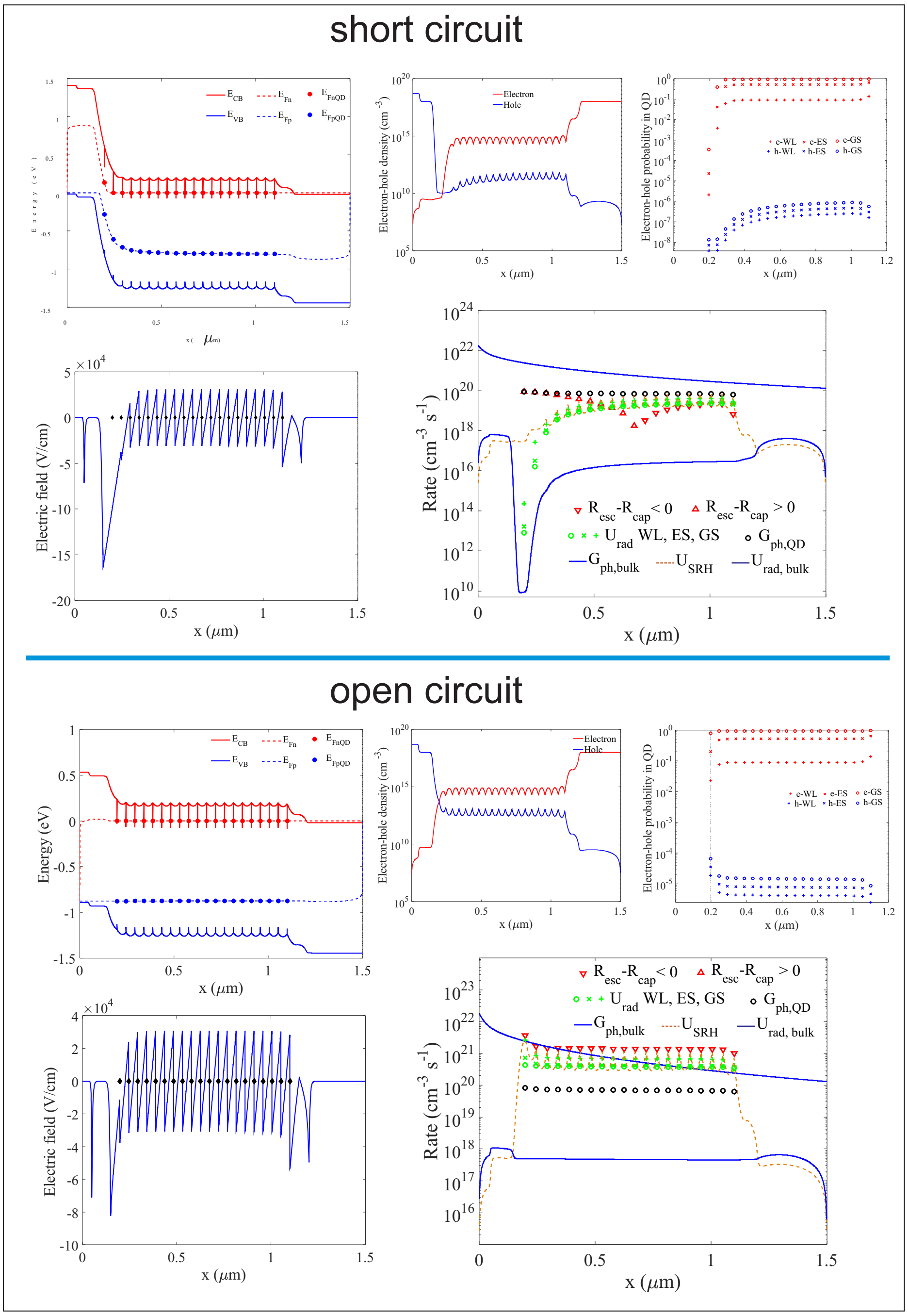

Figure S6: Spatial distribution at short circuit condition of energy bands (a), free carriers density (b), QD occupation probability (c), electric field (d), recombination rates (e). Spatial distribution at open circuit condition of energy bands (f) , free carriers density (g), QD occupation probability (h), electric field (i), recombination rates (j). Diamond symbols in the electric field figures (d) and (i) indicate the QD layers position.

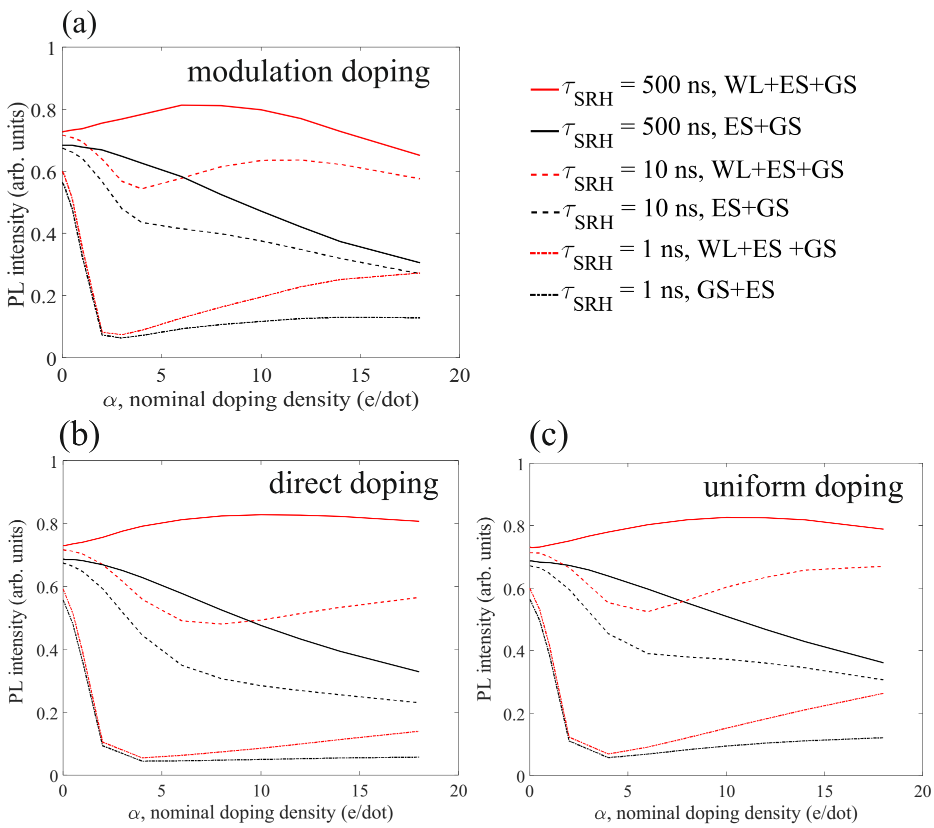

Figure S7: Variation of the integrated PL intensity (IPL) at open circuit condition as a function of the nominal doping density, under the hypothesis of different SRH recombination lifetime, for the three doping methods: (a) modulation doping, (b) direct doping, (c) uniform doping. Red lines correspond to the total IPL, integrated over WL, ES and GS emission, while black lines single out the contribution of ES and GS only.