Support information

(Dated: August 8, 2012)

To see more detail concerning the effect of γ on the yield, in Fig. 1 we examine the yield variation upon changing γ and m together. In addition to the slope of the line shape to the left side and the position of the peak value far from the middle of the band, the peak values with the same m drop with γ (compare the different panels). Inside the same panel, the yield increases with m because of more population tunneling from site 0 to site 1 and through the acceptor sites to the electrode.

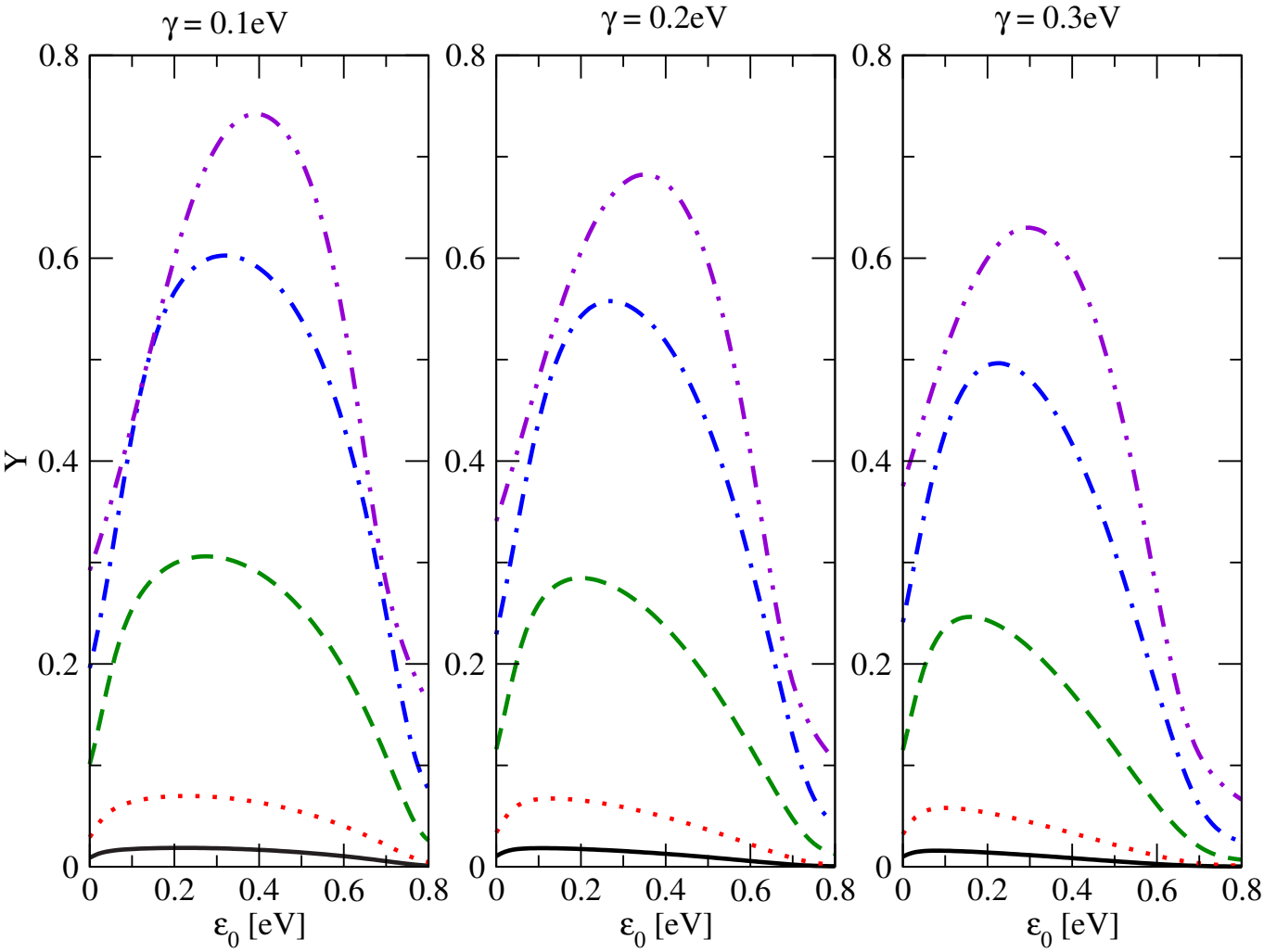

FIG. 1: Yield Y of charge separation shown as a function of ε_0 obtained with different charge trapping parameter γ and coupling parameter m. N = 60, $\eta = 0.05eV$, $b = 0.2eV$, $m = 0.01eV$ (black line); $m = 0.02eV$(dotted line); $m = 0.05eV$(dashed line); $m = 0.1eV$(dotted+dashed) and $m = 0.2eV$(double dotted+dashed), $\gamma = 0.1eV$ (left panel); $\gamma = 0.2eV$ (middle panel) and $\gamma = 0.3eV$ (right panel).

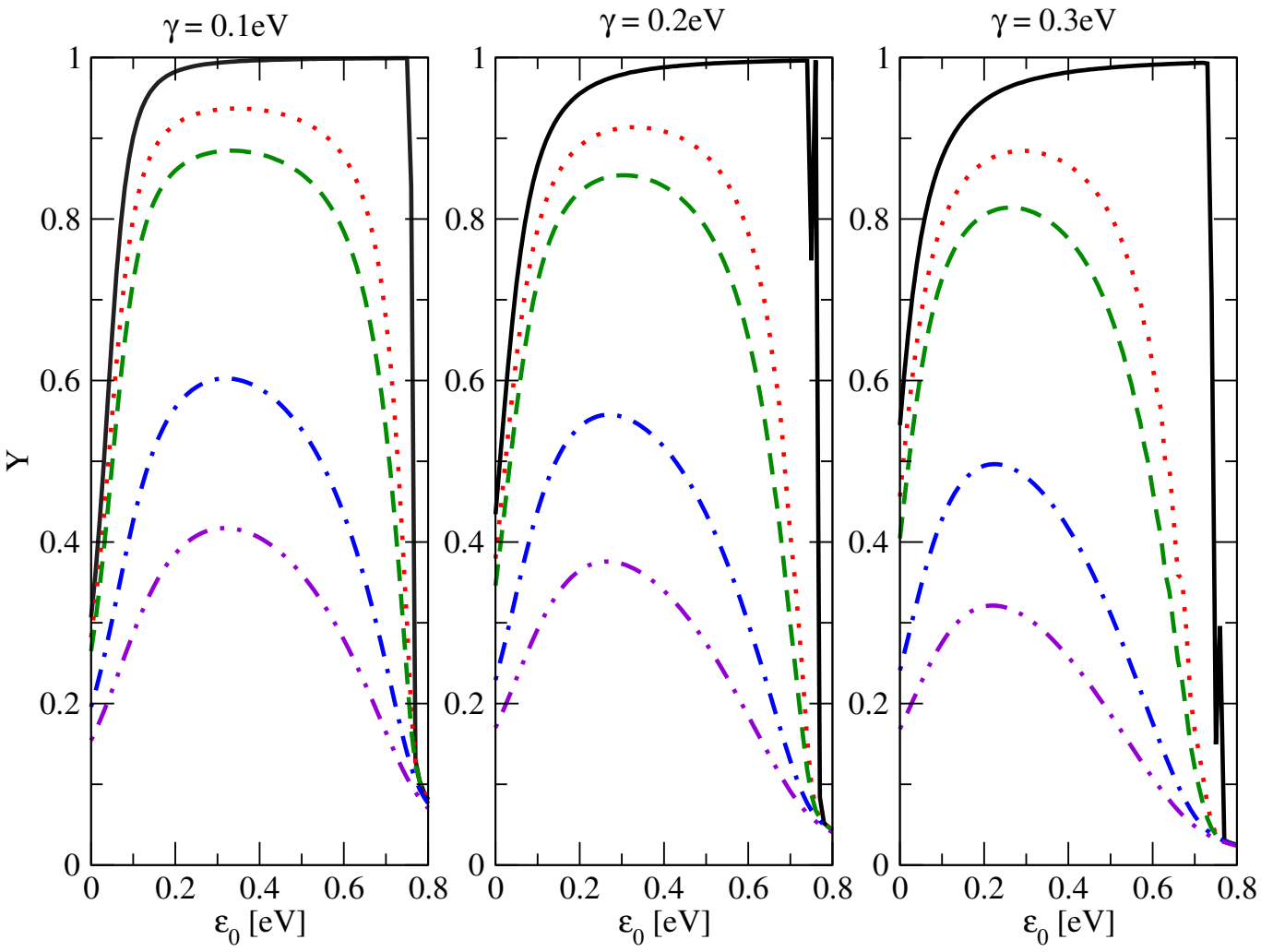

FIG. 2: Yield Y of charge separation shown as a function of ε_0 with different charge trapping parameter γ and decay parameter η. N = 60, $m = 0.1eV$, $b = 0.2eV$, $\eta = 0$ (black line); $\eta = 0.005eV$(dotted line); $\eta = 0.01eV$(dashed line); $\eta = 0.05eV$(dotted+dashed) and $\eta = 0.1eV$(double dotted+dashed), $\gamma = 0.1eV$ (left panel); $\gamma = 0.2eV$ (middle panel) and $\gamma = 0.3eV$ (right panel).

Figs. 2 shows the influence of changing γ and η together. In addition to changes in the line shape, the width with the same η decreases with γ (compare the different panels). Inside the same panel, the yield decreases with η because more population transfers back to the ground state through the radiationless process inside the donor.

In Fig. 3 the site number N changes from 4 to 80, and the central gap of the $1 - P_O$ vs ε_0 line becomes narrower as N $\rightarrow$ 80. When N is larger than 16, the line shapes mostly have no change. By diagonalizing the Hamiltonian of a isolated system including only the acceptor part, we will get an energy band from $-|2b|$ to $|2b|$. Then the system can be taken as the single donor site coupling to

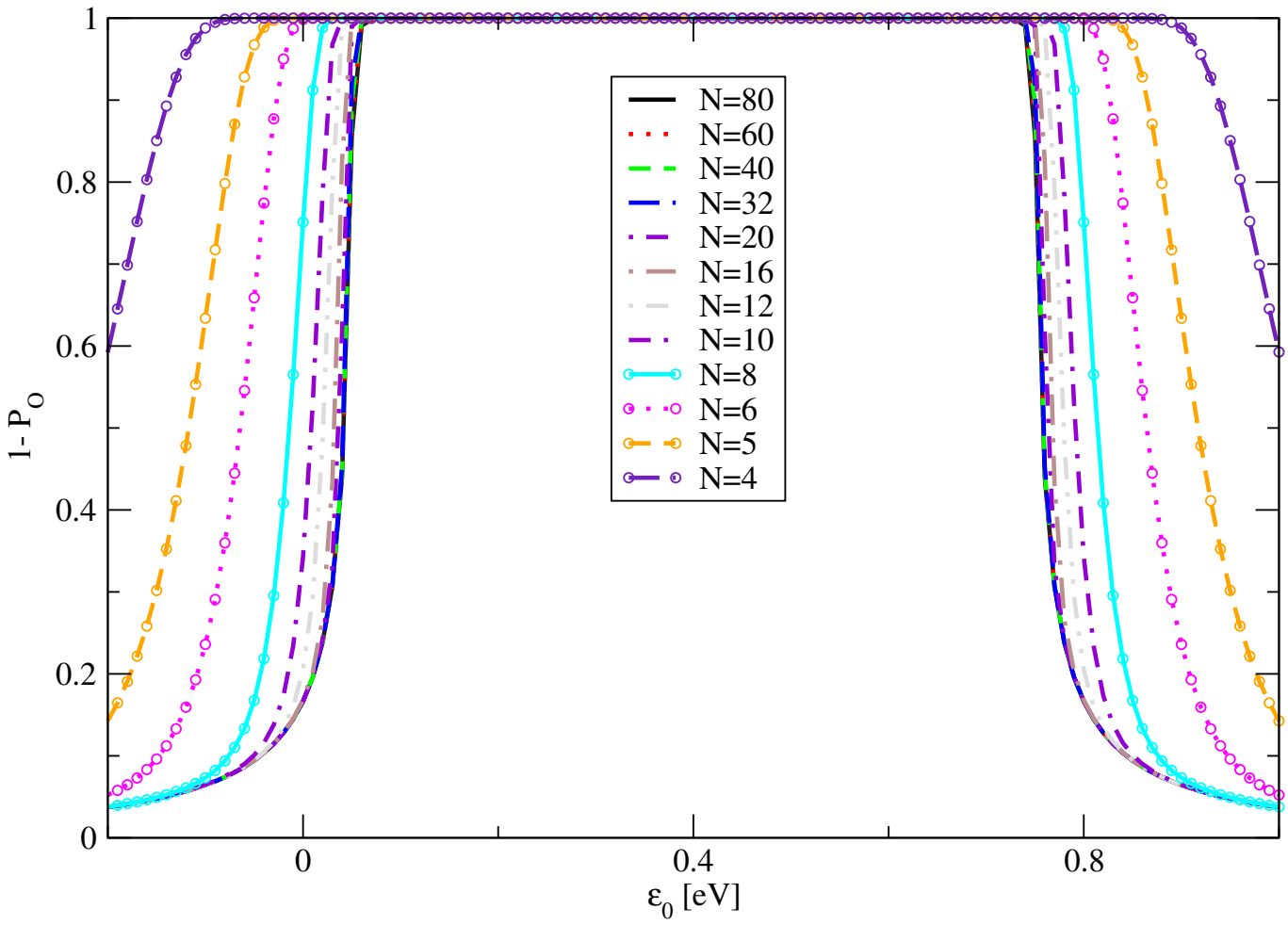

FIG. 3: In long time limit total population P_O shown as a function of ε_0 under different number site N. $\gamma = 0.0$, $b = 0.2eV$, $m = 0.1eV$, $\eta = 0$. (In this figure $1 - P_O$ is shown).

such a energy band. The central gap of the $1 - P_O$ vs ε_0 line will be shorter than $4b$ because of the coupling parameter m.