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Analytical Study on Piezoelectric Effects on Exciton Dissociation

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Abstract. We analytically and numerically compute the Onsager dissociation rate (exciton dissociation) on an interface induced by a piezoelectric potential in an inorganicorganic hybrid p-n junction system (ZnO + (poly(p-phenylene vinylene)); PPV). When a positive piezoelectric potential is created at the interface region owing to the deformation of the system, free electrons accumulate at the interface. Hence, screening effects are observed. It is assumed that the electron layer formed at the interface then attracts free holes from the p-type PPV region, which leads to exciton formation, possibly via the Langevin recombination process. The increased exciton density can then contribute to the Onsager dissociation rate, which is maximum around the interface. This paper focuses on the role of piezoelectric effects in promoting exciton formation at the interface and its relation with the exciton dissociation rate.

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1 Introduction

Dissociation of bounded electron-hole pairs (excitons) is important in organic solar cell devices [1, 2]. In a p-n junction system, a photo-generated exciton can migrate to the interface via diffusion. Then, owing to the potential difference (built-in potential plus applied bias) between each side of the interface, exciton dissociation, resulting in charge separation, can occur across the interface [1, 2]. Here, the dissociation of excitons can

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be explained by Onsager's theory [3,4], where the dissociation rate constant (k_{diss}) [5] is given by,

$$k_{diss}=\frac{\gamma}{\frac{4}{3}\pi a^3}e^{-E_b/k_BT}\left[1+b+\frac{b^2}{3}+\frac{b^3}{18}+\frac{b^4}{180}+\cdots\right]. \tag{1.1}$$

In Eq. (1.1), E_b is the exciton binding energy, $b=q^3|\vec{\nabla}\varnothing|/8\pi\epsilon k_B^2T^2$ is the field parameter, k_B is the Boltzmann constant, T is the temperature, γ is the Langevin recombination parameter, given by $\frac{q}{\epsilon}(\mu_n+\mu_p)$ [6] and a is the electron-hole pair distance. Then, the Onsager dissociation rate D [3,4] is given by,

$$\begin{aligned} D&=k_{diss}\cdot X \qquad (1.2)\\ &=\frac{\gamma}{\frac{4}{3}\pi a^3}e^{-E_b/k_BT}\left[1+b+\frac{b^2}{3}+\frac{b^3}{18}+\frac{b^4}{180}+\cdots\right]X, \qquad (1.3)\end{aligned}$$

where X is the exciton density.

The calculation of D requires various parameters such as b, X, γ, E_b, a, k_B and T. Among them, the field parameter b is associated with the electric field, which is related to the piezoelectric field/potential induced at the p-n interface in the hybrid junction system when the system is deformed.

In this case, electrons or holes around the interface can accumulate at the interface, if the piezoelectric field is strong enough even a depletion zone is formed. The piezoelectric charges resulting in piezoelectric fields are not newly created ones but are resulted from an occurrence of non-zero dipole moments which are generated by the deformation of the structures of the piezoelectric materials using the external forces exerted onto the system. (There is no change in total number of charges). Around such piezoelectric charges generated, free carriers can be accumulated into them and screen them to reduce the piezoelectric potential or can conserve them to maintain the piezoelectric potential.

Excitons can be formed via the exciton recombination process (Langevin recombination) [7,8], by controlling the free carriers collected at the interface, resulting from the piezoelectric potential induced. In this way, the density of excitons (and ultimately, the dissociation rate) can be controlled, as the piezoelectric field can affect both b and X. This is a point of modeling excitons here, but there are yet no experimental papers measuring such a phenomenon of exciton formation induced by the piezoelectric effects in a hybrid p-n junction system.

In this paper, we first analytically solve the Onsager dissociation rate in the inorganicorganic hybrid p-n junction structure where a positive piezoelectric potential is generated on the p-n interface, which leads to accumulation of electrons that then assist in forming excitons. These excitons are then dissociated into free carriers. We calculate the Onsager dissociation rate numerically to better understand the piezoelectric effects on the exciton dissociation in the hybrid p-n junction system and obtain a better physical insight into it.