# Supplementary Information for:

## Energetics of Exciton Binding and Dissociation in Conjugated Polymers: A Tight Binding Approach

Joel H. Bombile, Michael J. Janik, Scott T. Milner.

## Coulomb integral between two smeared charge distributions

We evaluate the Coulomb integral between two smeared charge distributions, represented as three-dimensional Gaussians given by

$$\rho(r) = q_0 \frac{e^{r^2/(2\sigma)^2}}{(2\pi\sigma)^{3/2}} \tag{1}$$

where $\sigma$ is the characteristic size (radius), and $q_0$ the elementary charge. The integral for such charge distributions located at site $i$ and $j$, $E_C(i,j)$, is given by

$$\begin{aligned} E_C(i,j) &= \int dr \int dr' \, \frac{\rho_i(r)\rho_j(r')}{|r-r'|} \\ &= \frac{1}{r}\text{erf}\left(\frac{r}{2\sigma}\right) \end{aligned} \tag{2}$$

where the latter result is obtained by evaluating the integral in Fourier space. Evidently $E_C(i,j)$ only depends on the distance $r$ between sites $i$ and $j$, and the characteristic width $\sigma$ of the smeared charge distribution $\rho$. Figure S1 displays this result as a dimensionless function of $r/\sigma$, in units of the energy scale $U_0 = q_0^2/(4\pi\epsilon_0\sigma)$. A deviation from the $1/r$ potential is seen for interactions involving smeared charges that are two sites or less apart.

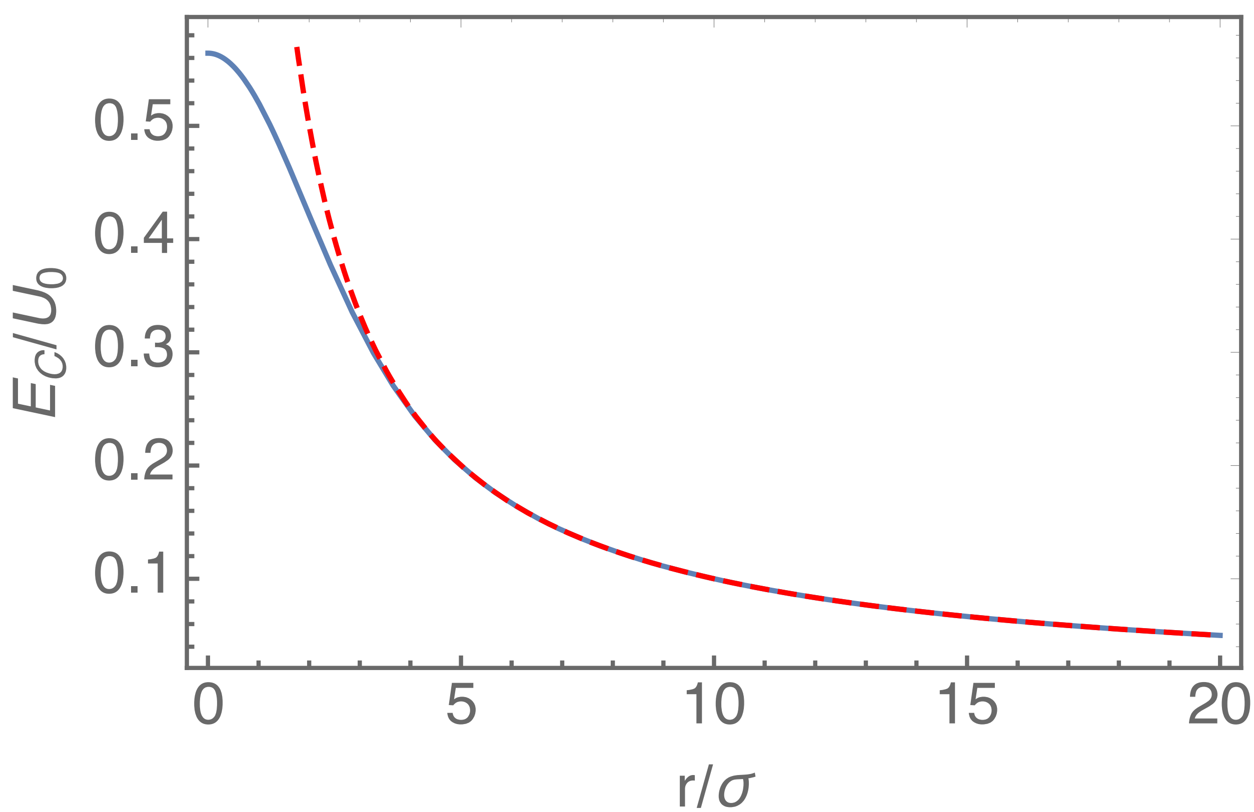


Figure S1: Interaction energy between two Gaussian charge distributions separated by $r$. Solid curve is Equation 2; dashed curve is $1/r$, valid at large separations.

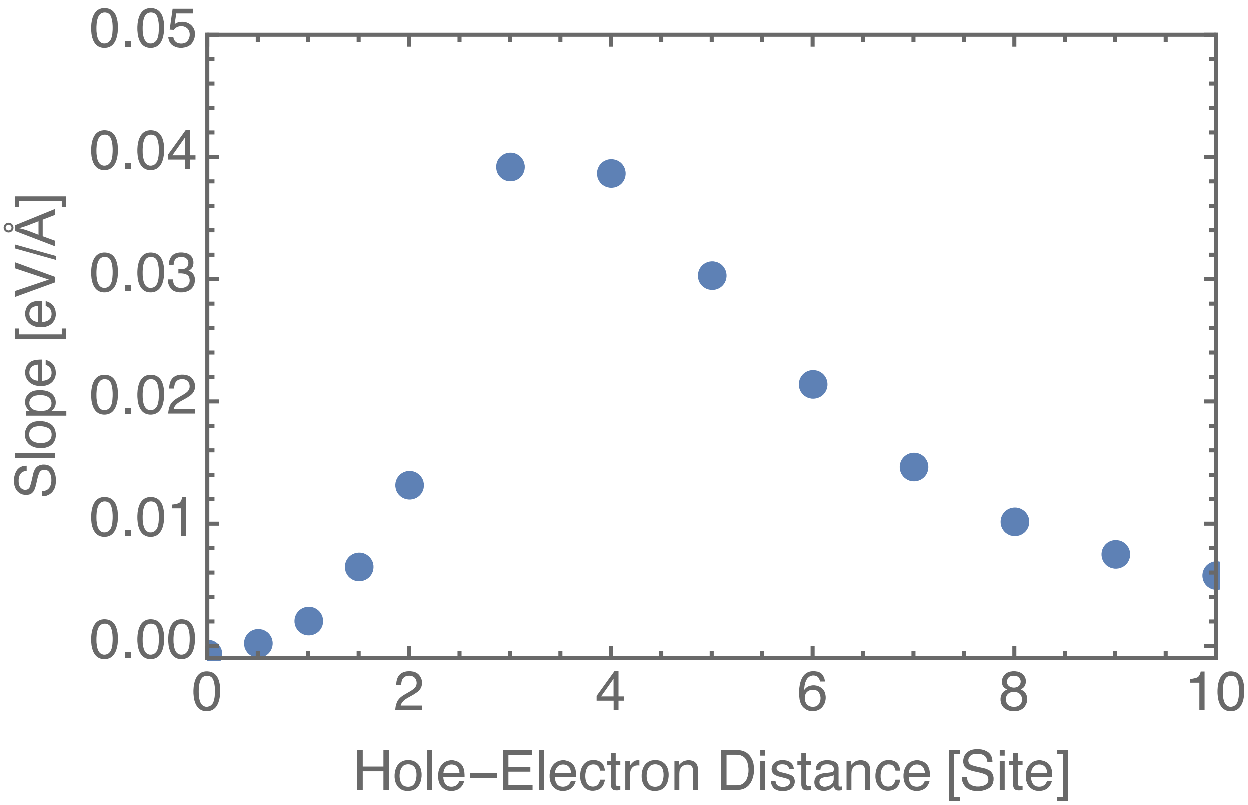


Figure S2: Attractive force (slope of bare Coulomb potential) between the two carriers as a function of hole-electron distance.