Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supporting Information for "Thermal Effect on Morphology and Performance of Organic Photovoltaics"

Eisuke Kawashima,[ab] Mikiya Fujii,[ab] and Koichi Yamashita*[ab]

[a] Department of Chemical System Engineering, Graduate School of Engineering, The University of Tokyo, Tokyo 113-8656, Japan.

[b] CREST, Japan Science and Technology Agency (JST), Tokyo 113-8656, Japan

S1 Reptation

S1.1 Results of Polymer/Small Molecule Volumetric Ratio of 1:1

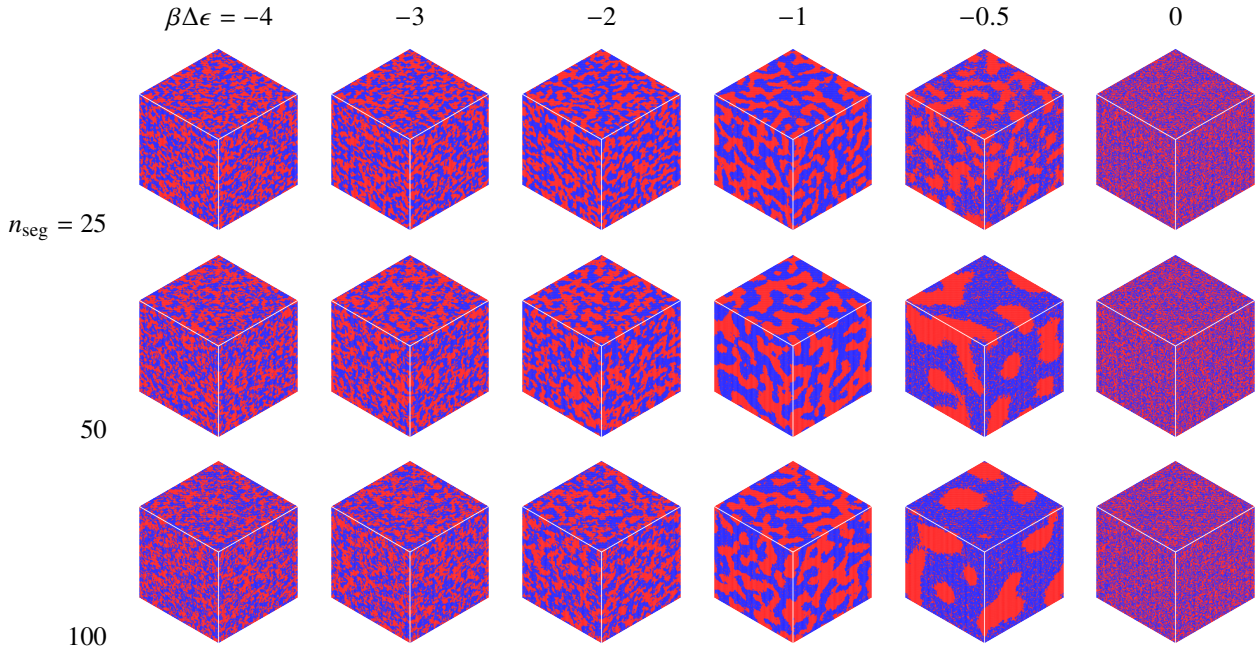

Fig. S1: Morphologies with number of segments $n_{\mathrm{seg}} = 25, 50, 100$; and $\beta\Delta\epsilon = -4, -3, -2, -1, -0.5, 0$. Blue and red sites represent polymers and small molecules, respectively.

S1.2 Results of Polymer/Small Molecule Volumetric Ratio of 1:2

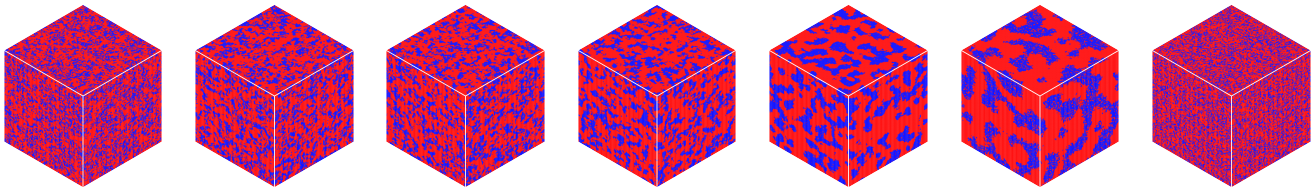

Fig. S2: An initial and generated morphologies. The number of polymer segments is set to 75. Blue and red sites represent polymers and small molecules, respectively.

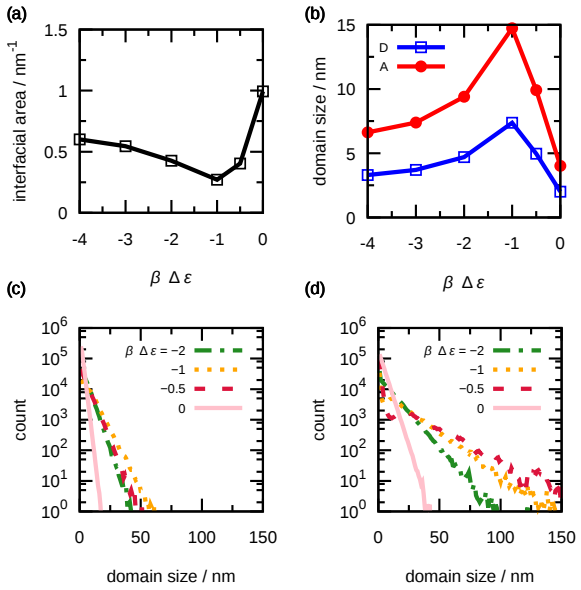

Fig. S3: $\beta\Delta\epsilon$ dependence of (a) interfacial area and (b) mean domain size of donor (D) and acceptor (A).

S2 Dynamic Monte Carlo

S2.1 Performance Parameters

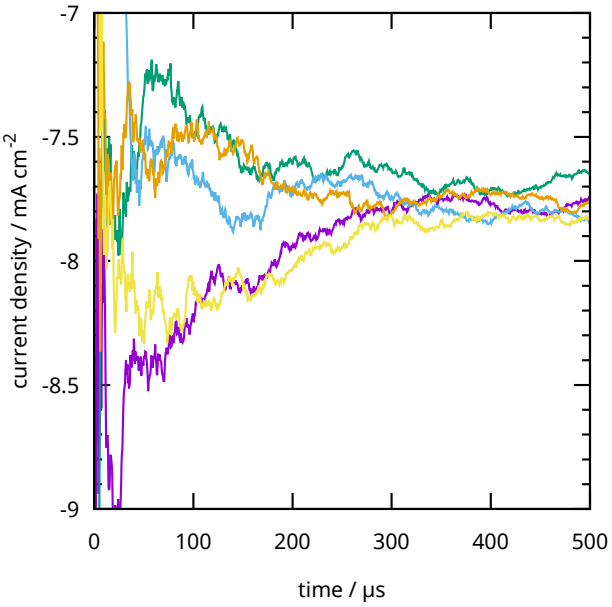

Fig. S4: Current density vs time of five independent simulation runs. The morphology is BHJ with $\beta\Delta\epsilon$ of −4, and applied voltage is 0. The first period (0–250 s) was discarded as "burn-in."

S2.2 Transient Absorption Spectroscopy

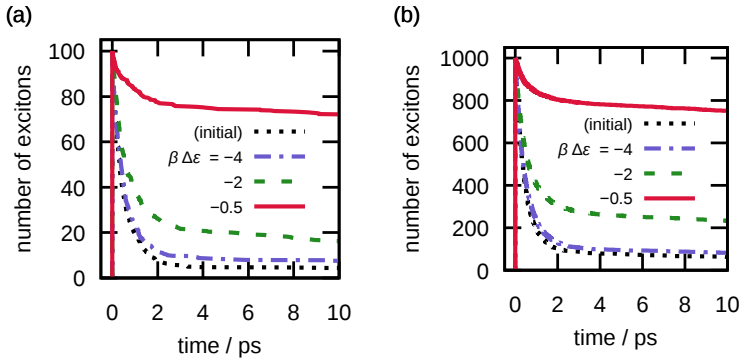

Fig. S5: Simulated number of excitons with initial number of (a) 100 and (b) 1000.

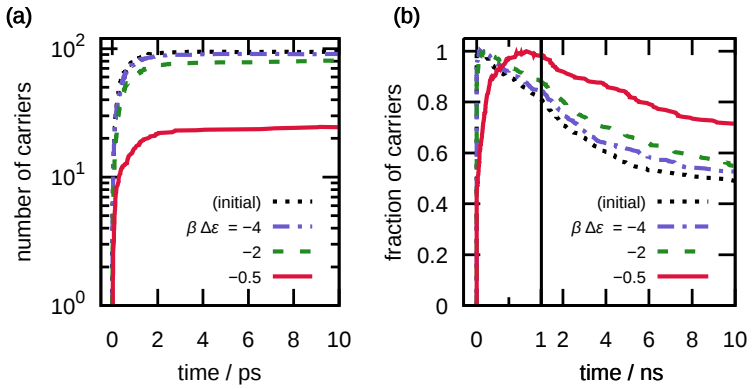

Fig. S6: Simulated charge (a) generation and (b) recombination dynamics of initial structure and morphologies with various $\beta\Delta\epsilon$. The number of initial excitons is 100.

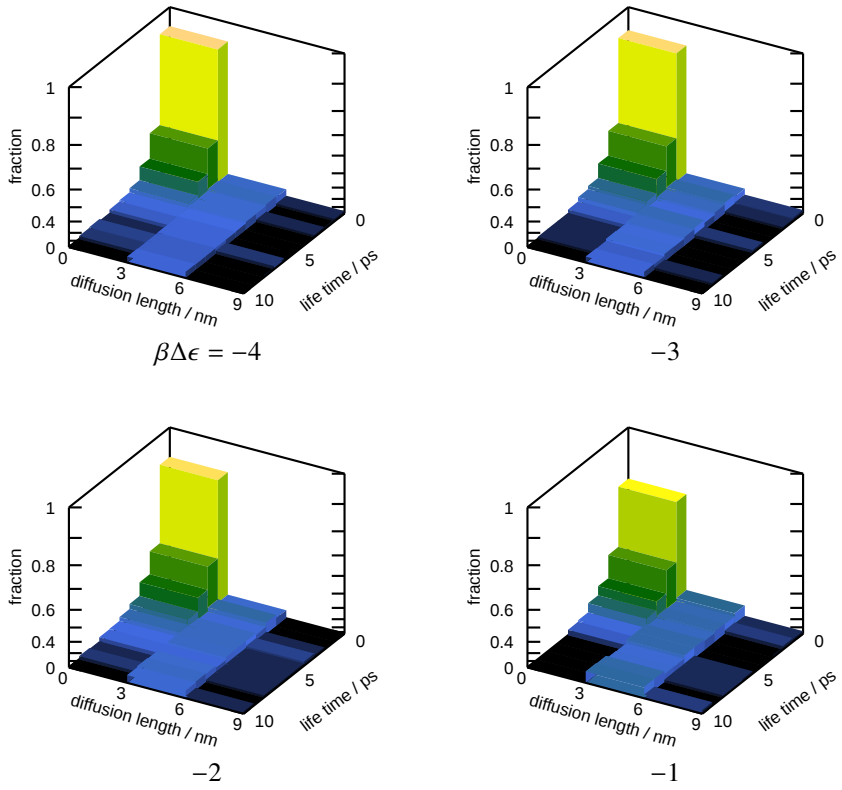

Fig. S7: Fraction of diffusion length and life time of dissociated excitons of each morphology. The number of initial excitons is 1000.

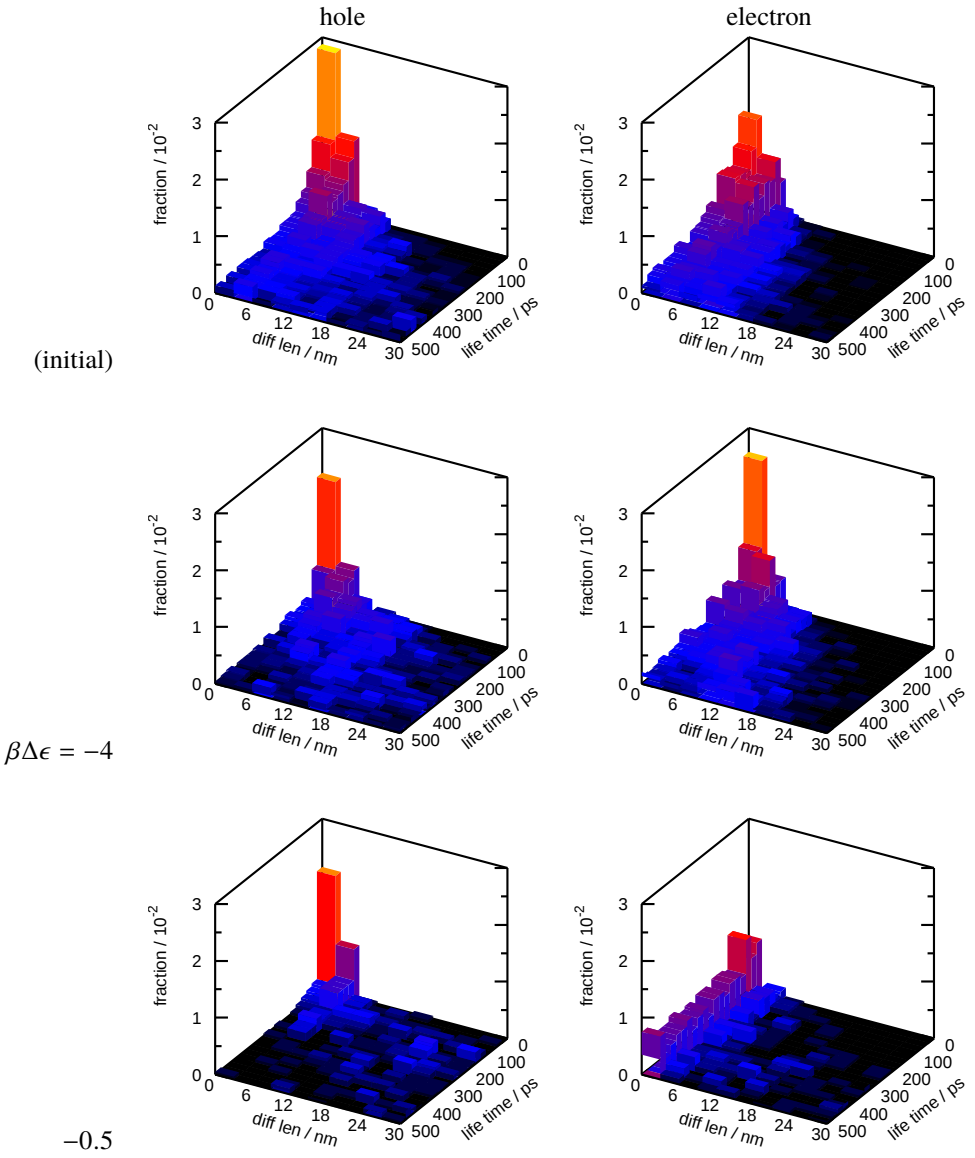

Fig. S8: Diffusion length and life time of the recombined holes and electrons. The number of initial excitons is 1000.