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**Morphological Effect on Performance of Organic Photovoltaics—In Terms of Entropy and Helmholtz Energy** EISUKE KAWASHIMA, MIKIYA FUJII, KOICHI YAMASHITA, Department of Chemical System Engineering, Graduate School of Engineering, the University of Tokyo and JST, CREST — Organic photovoltaics (OPVs) are promising alternatives to conventional silicon solar cells, but the current major challenge is their low performance. Morphology—phase separation and crystallinity of organic semiconductors—is a key factor to improve performance, and depends not only on materials but also on manufacturing processes, *e.g.*, thermal annealing. At present, however, optimization scheme of morphologies is not established. In our previous study, we examined temperature dependence of morphologies and effects of morphology on performance by device-scale simulations. Bulk heterojunction morphologies were generated by reptation, and current density–voltage characteristics and transient absorption spectroscopy were simulated by Dynamic Monte Carlo (DMC); we elucidated the existence of the optimal annealing temperature for efficiency.[1] In this presentation, we show Helmholtz energy $F$ and entropy $S$ of charge separation evaluated by graph theory and DMC simulations. We revealed that (i) $S$ drastically decreases $F$, (ii) $F$ attains a maximum at e–h distance of *ca.* 6 nm, and (iii) charge separation efficiency is determined by barrier height of $F$.

[1]E. Kawashima, *et al.*, *Phys. Chem. Chem. Phys.*, **2016**, 18, 26456–26465

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