Bicontinuous minimal surface nanostructures for polymer blend solar cells: Supporting information

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Generation of the novel structures

The double gyroid is a close structural model for the well-known gyroid phase in diblock copolymers,[?] a phase that had previously been identified as the double diamond.[?] The single gyroid is not found in diblock copolymers, but has been identified in linear terblock copolymers ([?] although not with volume fraction 50%), and as the nanostructure of the wings in certain butterfly species.[?] Black-and-white geometries with black representing the domain of the donor polymer and white the acceptor polymer can be generated from the gyroid and diamond triply-periodic minimal surfaces by two mechanisms. First a single geometry is derived by setting all voxels in one of the two labyrinthine domains to black, and those in the other domain to white, yielding a structure with 50% volume fraction of both domains. This procedure generates a partition of space into two identical domains. The single gyroid has symmetry group $I4_132$, and the single diamond $Fd\overline{3}m$. Second, double geometries are derived by setting all voxels within a given distance Δ from the minimal surface to black and all others to white. This procedure yields a partition of space into two network- or labyrinth-like white domains separated by a layer of black voxels (often termed the matrix). The volume fraction of black voxels can be adjusted by the choice of Δ. The symmetry group of the double gyroid is $Ia\overline{3}d$, and that of the double diamond $Pm\overline{3}m$.

Our binary datasets are obtained by generating surface patches representing $n \times n \times n$ cubic translational unit cells of the gyroid or diamond surface, using the Weierstrass parametrisation (see e.g.[?]). With a choice of $a = L/n$ for the lattice parameter a and a given box width L, this yields surfaces that divide the box $[0, L]^3$ into two intertwined labyrinth domains. We superpose a voxel grid of M^3 voxels (hence of voxel length L/M) over this box and adjust the voxel value to white or black according to the scheme detailed above (which for the double geometries involves the computation of the so-called Euclidean distance map). The data in this article is obtained for n=1,2,4,8; L=64 and M=64. All of the datasets have 50% volume fraction of both phases.

Results for 5 suns illumination

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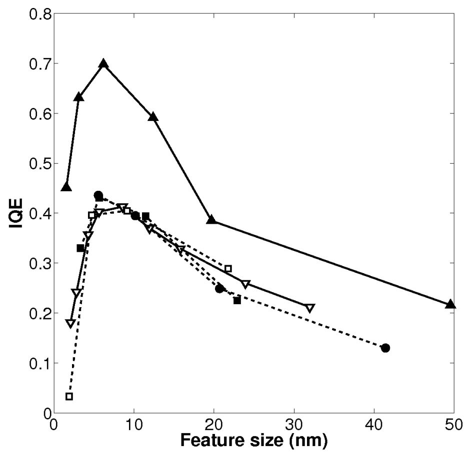

Figure S1: IQE as a function of feature size at 5 suns illumination for blends (solid line, ▽), rods (solid line, ▲), gyroids (dashed line, ●), double gyroid (dashed line, ■) and double diamond (dashed line, □).

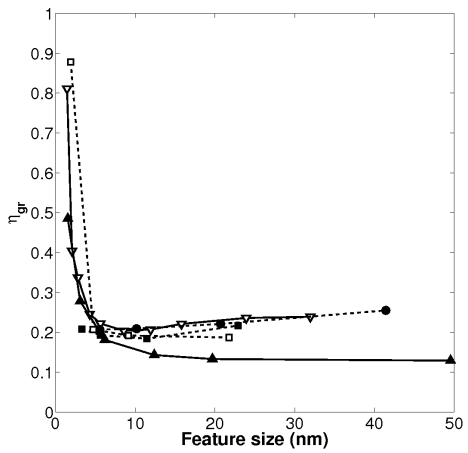

Figure S2: Geminate recombination at 5 suns for all morphology classes, as a function of feature size. Symbols and line types as for 1.

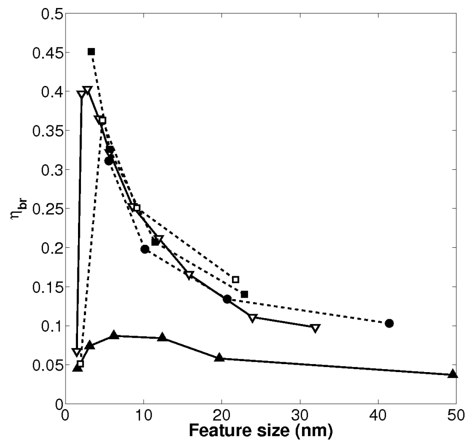

Figure S3: Bimolecular recombination at 5 suns for all morphology classes, as a function of feature size. Symbols and line types as for 1.