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 $\Delta$ 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 $\Delta$. 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.