

Description of Additional Supplementary Files

File name: Supplementary Data 1

Description: Initial atomic configurations for MD simulation of the J71:Y6 blend.

File name: Supplementary Data 2

Description: Optimized atomic configurations for MD simulation of the J71:Y6 blend.

File name: Supplementary Data 3

Description: Initial atomic configurations for MD simulation of the P3HT:Y6 blend.

File name: Supplementary Data 4

Description: Optimized atomic configurations for MD simulation of the P3HT:Y6 blend.

File name: Supplementary Data 5

Description: Initial atomic configurations for MD simulation of the PTB7:Y6 blend.

File name: Supplementary Data 6

Description: Optimized atomic configurations for MD simulation of the PTB7:Y6 blend.