Supporting Information for: P3HT:DiPBI bulk heterojunction solar cells: morphology and electronic structure probed by multiscale simulation and UV/vis spectroscopy

Thorsten Winands[1*], Marcus Böckmann[1], Thomas Schemme[2], Phong-Minh Timmy Ly[1], Djurre H. de Jong[3], Zhaohui Wang[4], Cornelia Denz[2], Andreas Heuer[3], Nikos L. Doltsinis[1]

[1] *Institut für Festkörpertheorie, Westfälische Wilhelms-Universität Münster and Center for Multiscale Theory & Computation, Wilhelm-Klemm-Str. 10, 48149 Münster, Germany.*

[2] *Institut für Angewandte Physik, Westfälische Wilhelms-Universität Münster, Corrensstr. 2/4, 48149 Münster, Germany.*

[3] *Institut für Physikalische Chemie, Westfälische Wilhelms-Universität Münster and Center for Multiscale Theory & Computation, Corrensstr. 28/30, 48149 Münster, Germany.*

[4] *Beijing National Laboratory for Molecular Sciences, Institute of Chemistry, Chinese Academy of Sciences Beijing, 100190, P. R. China*

(Dated: January 8, 2016)

* corresponding author, email: t.winands@wwu.de

Contents

1. COARSE GRAINED FORCE FIELD

bond type	r_0 [nm]	k [kJ/(mol·nm)]
TC1–TC1	0.186	constraint
TC1–TC2	0.197	constraint
TC1–SC2	0.47	1250
SC1–SC2	0.47	1250
DUM–DUM	0.375	25000

TABLE S1: Bond parameters of the Martini force field representation of P3HT: r_0 is the reference bond length and k the harmonic force constant.

angle type	ϕ_0 [°]	k [kJ/(mol· rad^2)]
TC2–TC1–SC2	180	25.0
DUM–DUM–DUM	160	35.0
TC1–TC1–DUM	155	135

TABLE S2: Angle parameters of the Martini force field representation of P3HT: ϕ_0 is the reference angle and k the harmonic force constant.

bond type	r_0 [nm]	k [kJ/(mol·nm)]
SC1–SC1	0.450	1250
SP3–SC1	0.320	1250
SP3–TC4	0.270	50000
TC4–TC4	0.270	50000

TABLE S3: Bond parameters of the Martini force field representation of DiPBI: r_0 is the reference bond length and k the harmonic force constant.

I–J	C6 [nm]	C12 [kJ/(mol)]
TC4–TC4	0.387	4.3
TC4–TC2	0.4335	4.2
TC4–TC1	0.4335	4.2
TC2–TC2	0.320	3.5
TC2–TC1	0.320	3.5
SC2–SC2	0.430	2.625
SC2–SC1	0.430	2.625
SC2–TC1	0.430	2.625
SC2–TC2	0.430	2.625
SC2–TC4	0.430	2.625
SC2–SP3	0.430	2.025
SC2–SC1	0.430	2.625
SC1–TC1	0.430	2.625
SC1–TC2	0.430	2.625
SC1–TC4	0.430	2.325
SC1–SP3	0.430	1.725

TABLE S4: Selected non-bonded parameters of the Martini force field. I and J are the bead types involved, C6 and C12 are the Lennard-Jones parameters.

2. DIPBI ATOMISTIC FORCE FIELD

See electronic topology file 'dipbi.top' in the ESI.

3. RADIAL DISTRIBUTION FUNCTION (RDF)

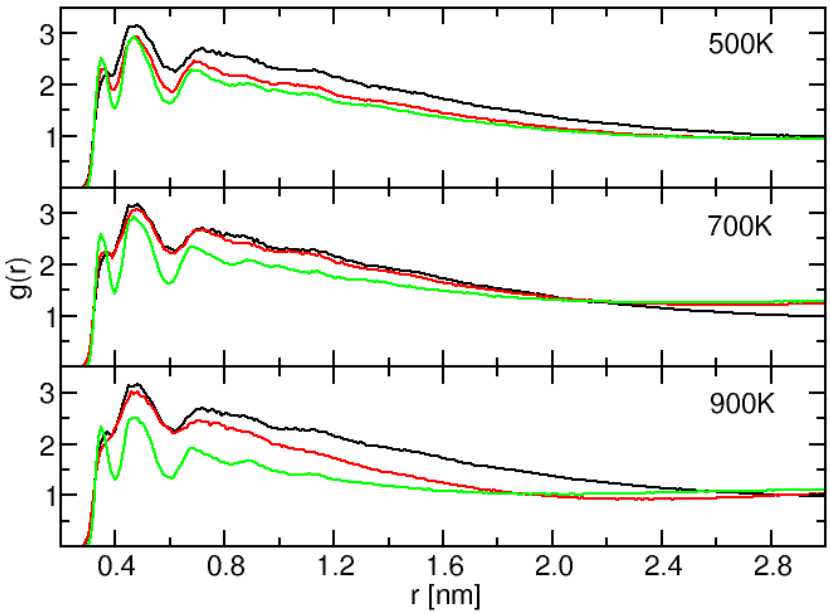

FIG. S1: Radial distribution function of the mixture for 500K, 700K and 900K. The black line represents the start configuration, the red line the 1 μs heated up mixture and the green line the structure cooled down to 300K.

4. DIHEDRAL ANGLE DISTRIBUTION OF P3HT

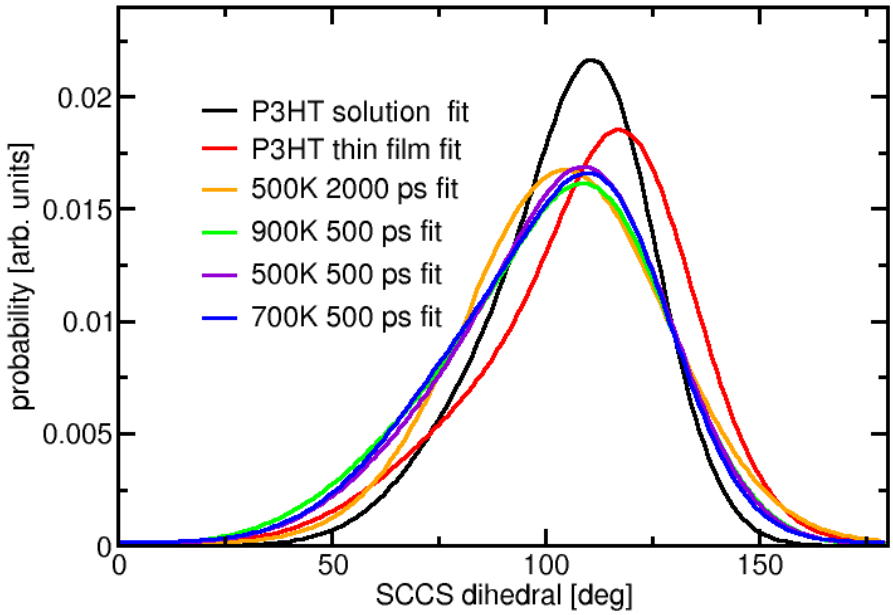

FIG. S2: Distribution of SCCS angles of the P3HT polymer after a double peak Gaussian fit. For the 500 K simulation, a slight structural relaxation is visible after 2000 ps.

5. TIME-DEPENDENT DOMAIN SIZES

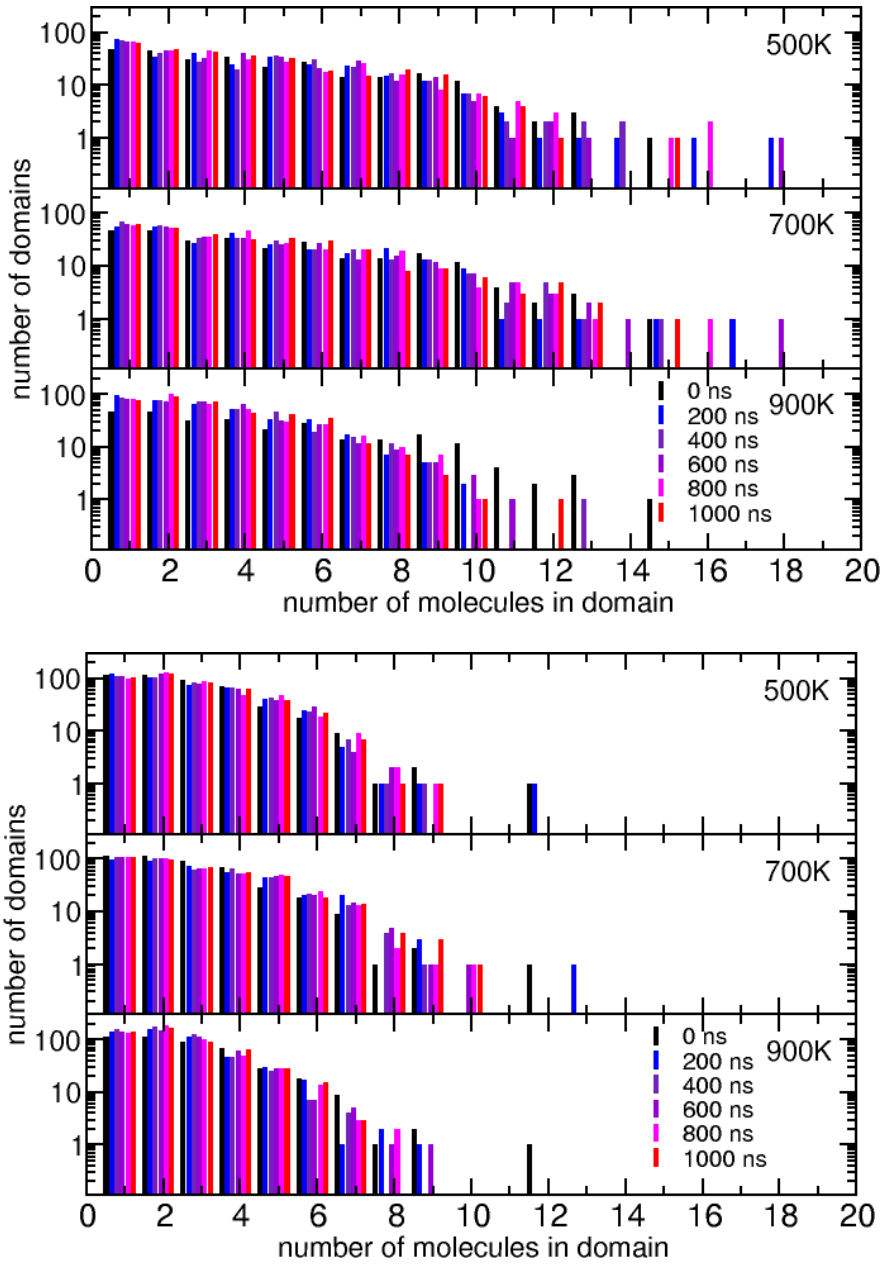

FIG. S3: Domain sizes of DiPBI calculated after different times with method 1 (top) and method 2 (bottom).

6. TIME-AVERAGED DOMAIN SIZES

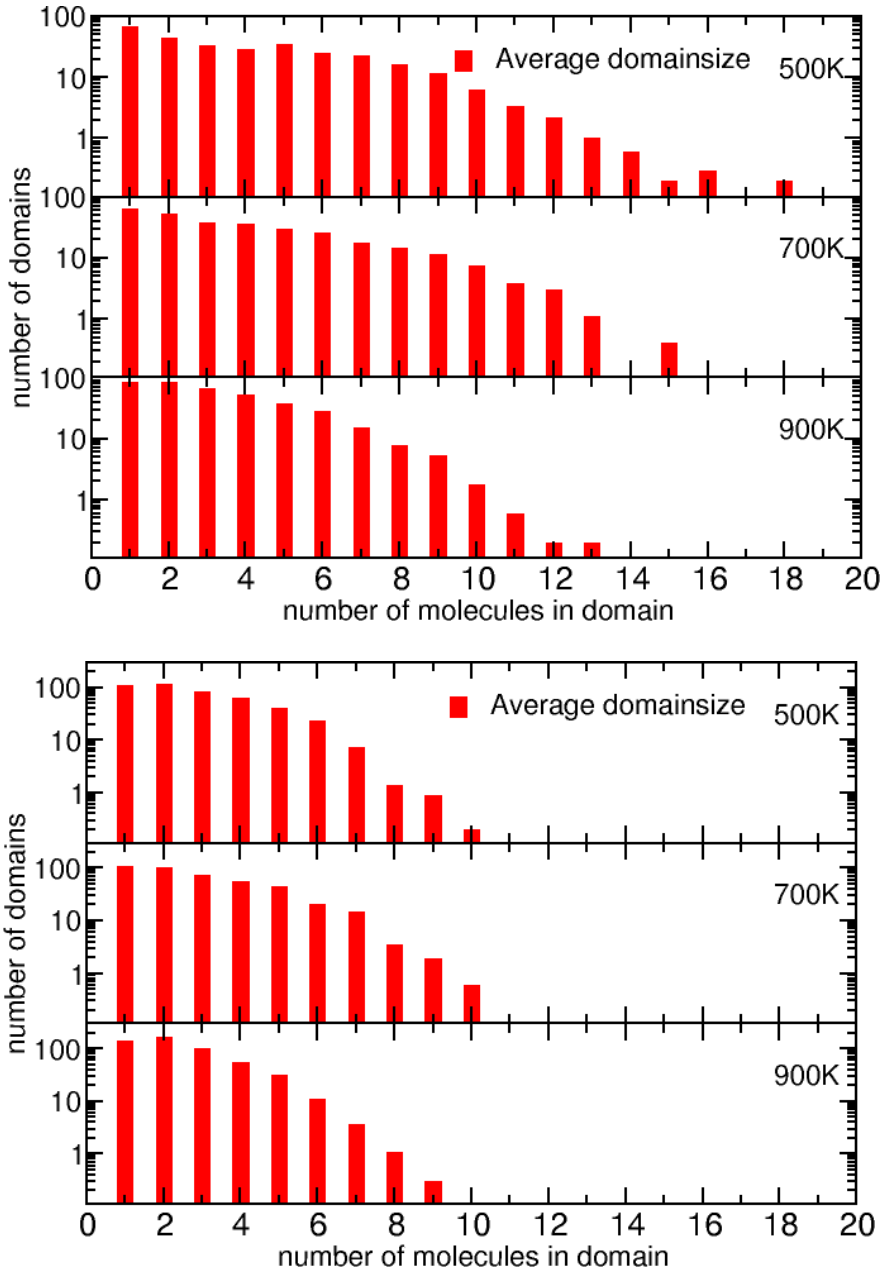

FIG. S4: Average domain sizes of DiPBI calculated with method 1 (top) and method 2 (bottom).

7. EFFECT COOLING RATE ON DOMAIN SIZES

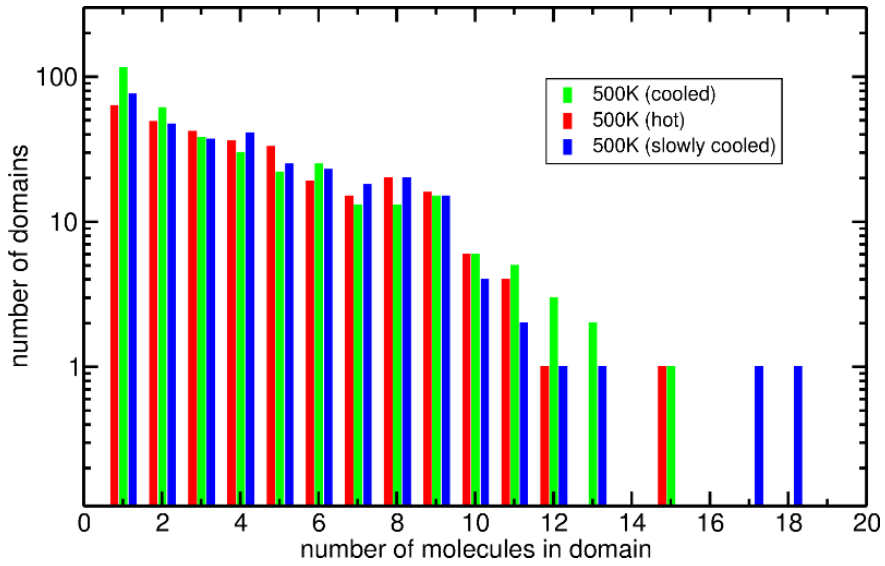

FIG. S5: Average domain sizes of DiPBI calculated with method 1 (top) and method 2 (bottom).

8. ABSORPTION SPECTRA OF OPTIMIZED STRUCTURES

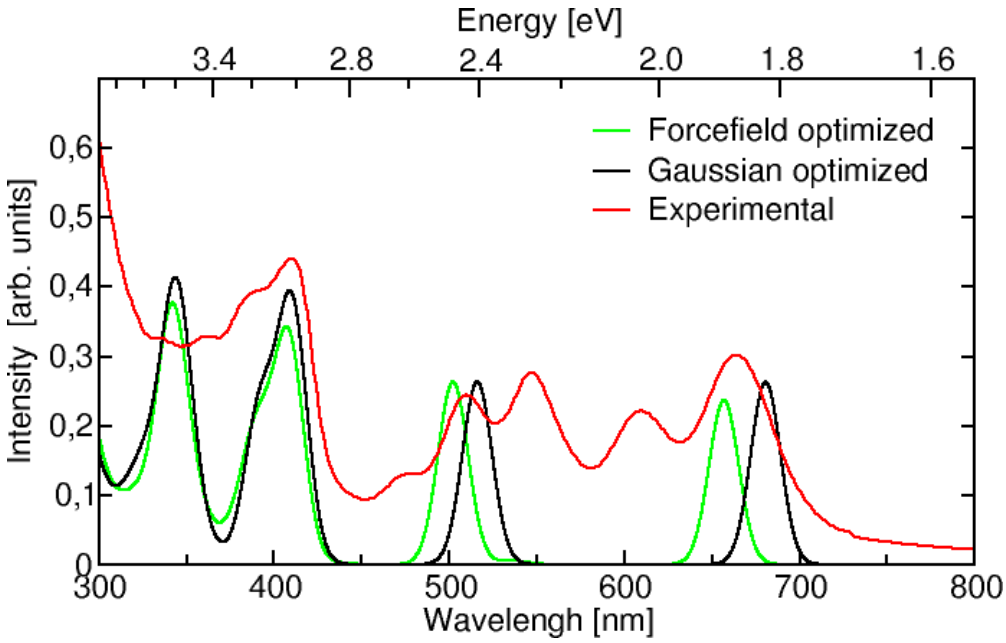

FIG. S6: Spectra of force field and Gaussian (PBE0/6-31G*) optimized structures in comparison to experimental data.

9. HYDROGEN BOND ANALYSIS

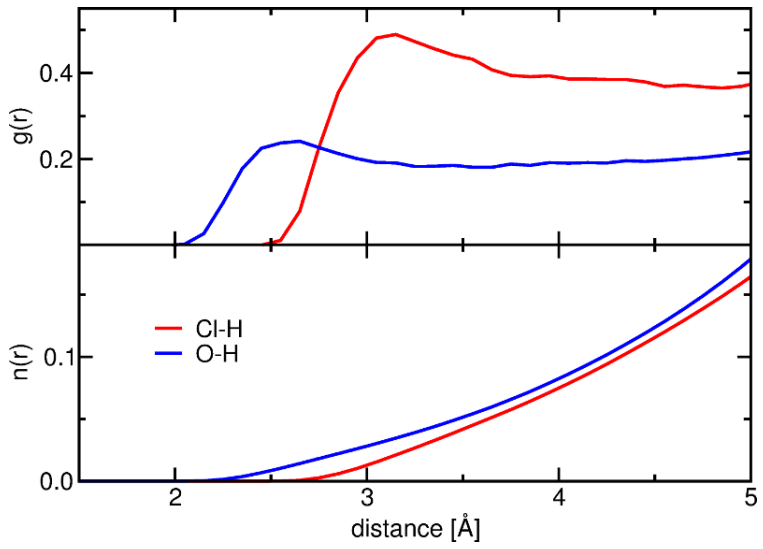

FIG. S7: Top: Cl...H and O...H radial distribution functions between DiPBI and P3HT molecules. Bottom: Corresponding coordination numbers.

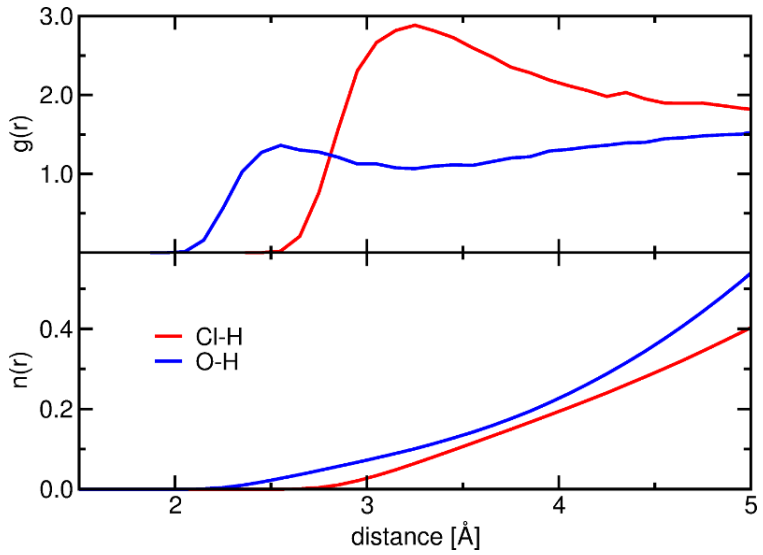

FIG. S8: Top: Cl...H and O...H radial distribution functions between DiPBI and DiPBI molecules. Bottom: Corresponding coordination numbers.