Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics

Modelling of P3HT:PCBM interface using coarse-grained forcefield derived from accurate atomistic forcefield

Supplementary information

A. Coarse-grained P3HT Forcefield

A.1. Forcefield

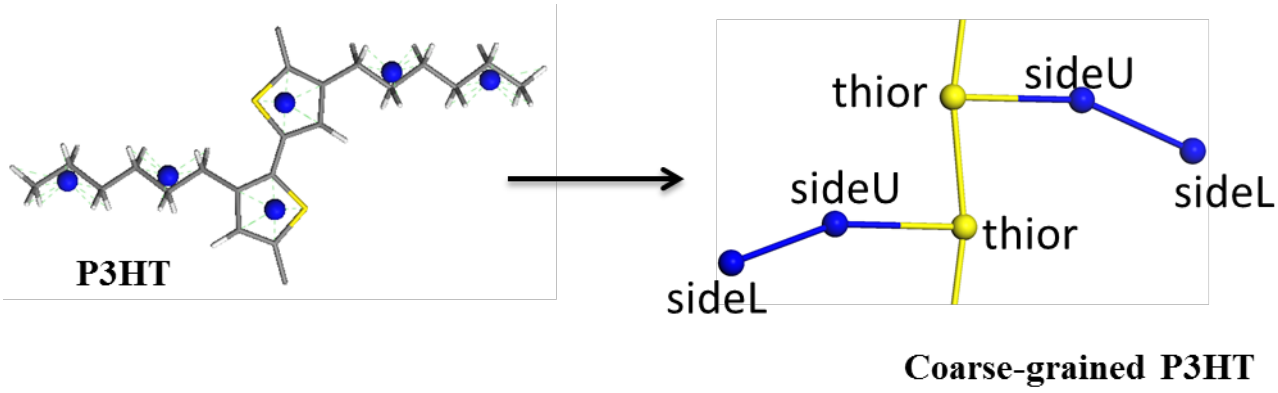

Figure. A1. Forcefield type notations for coarse-grained P3HT system used in this work

Forcefield Type	ϵ (kcal·mol^{-1})	σ (Å)	q (e)
thior	0.4368	3.385	-0.1087
sideU	0.2948	4.517	0.0957
sideL	0.3182	4.287	0.0129

Table. A1. Diagonal Van der Waals parameters and charges. The corresponding off diagonal VDW terms are derived therfrom following geometric mixing rules.

i	j	k_{bonds} (kcal·mol^{-1}·Å^{2})	r_0 (Å)
sideU	sideL	633.57	3.861
thior	sideU	2015.05	4.143
thior	thior	925.61	3.924

Table. A2. Bond stretching parameters

i	j	k	k_{angle} (kcal·mol^{-1}·rad^{-2})	θ_0 (degree)
sideL	sideU	thior	448.25	157.74
thior	thior	sideU	505.58	110.08
thior	thior	thior	542.08	171.38

Table. A3. Angle bending parameters

i	j	k	l	V_1(kcal·mol^{-1})	V_2(kcal·mol^{-1})	V_3(kcal·mol^{-1})	V_4(kcal·mol^{-1})
sideU	thior	thior	sideU	-3.9697	9.1853	-1.7845	2.4383

Table. A 4. Torsion parameters

A.2. Fitting of Short Range Interaction

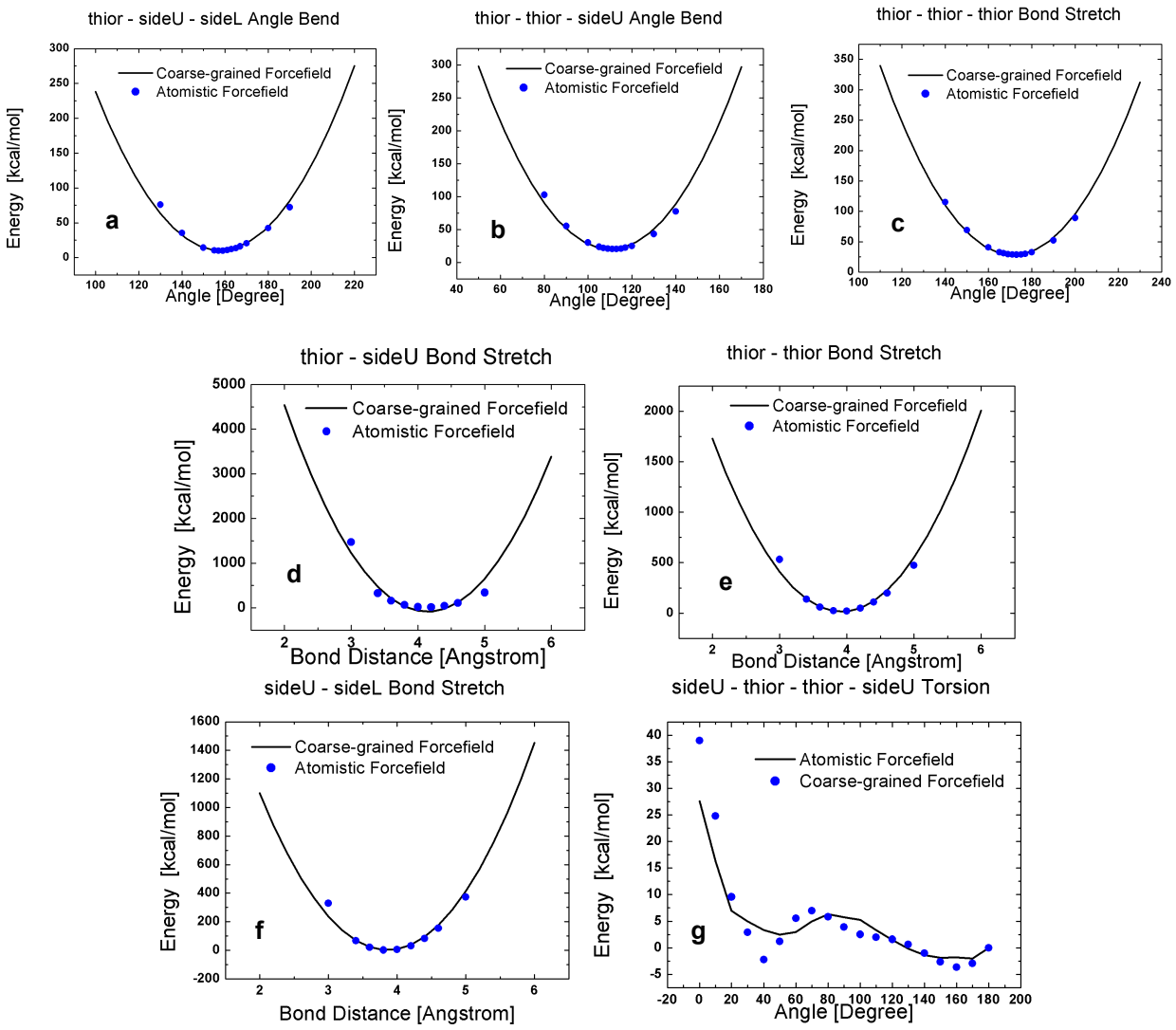

Figure. A2. Fitting against atomistic forcefield was used to obtain short range interaction parameters for coarse-grained forcefield. Here fitting results for all interaction contributions are shown with angle bending terms: a) thior-sideU-sideL, b) thior-thior-sideU and c) thior-thior-thior; bond stretching terms: d) thior-sideU, e) thior-thior and f) sideU-sideL; and torsion term: g) sideU-thior-thior-sideU

B. Coarse-grained PCBM Forcefield

B.1. Forcefield

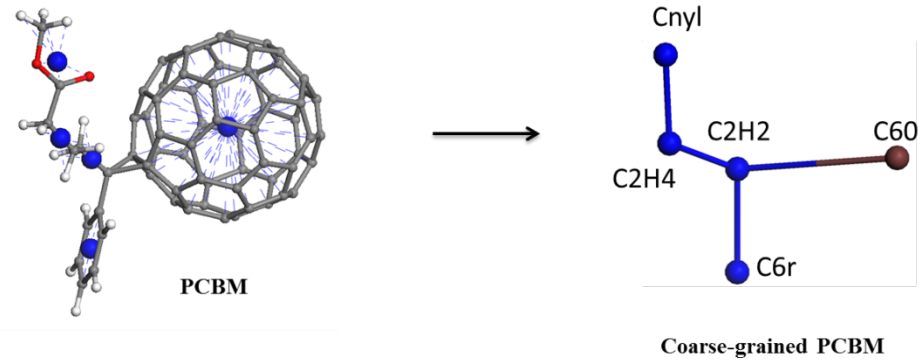

Figure. B1. Forcefield type notations for coarse-grained P3HT system used in this work

Forcefield Type	ϵ (kcal·mol^{-1})	σ (Å)	q (e)
C2H2	0.14784	5.438	-0.0280
C2H4	0.19404	5.456	0.1060
C60	3.234	9.355	0.0301
C6r	0.4389	3.763	-0.1555
Cnyl	0.47047	6.650	0.0474

Table. B5. Diagonal Van der Waals parameters and charges. The corresponding off diagonal VDW terms are derived therfrom following geometric mixing rules.

i	j	k_{bonds} (kcal·mol^{-1}·Å^2)	r_0 (Å)
C2H4	C2H2	526.53	2.579
C2H4	Cnyl	853.38	2.963
C60	C2H2	1202.30	5.573
C6r	C2H2	641.85	3.481

Table. B6. Bond stretching parameters

i	j	k	k_{angle} (kcal·mol^{-1}·rad^{-2})	θ_0 (degree)
C2H2	C2H4	Cnyl	519.67	117.32
C60	C2H2	C2H4	1948.96	126.86
C6r	C2H2	C2H4	565.19	115.67
C6r	C2H2	C60	8984.41	100.37

Table. B7. Angle bending parameters

i	j	k	l	V_1(kcal·mol^{-1})	V_2(kcal·mol^{-1})	V_3(kcal·mol^{-1})	V_4(kcal·mol^{-1})
Cnyl	C2H4	C2H2	C60	-57.7995	-29.0456	-5.3513	-6.092

Table. B8. Torsions parameters

B.2. Fitting of Short Range Interaction

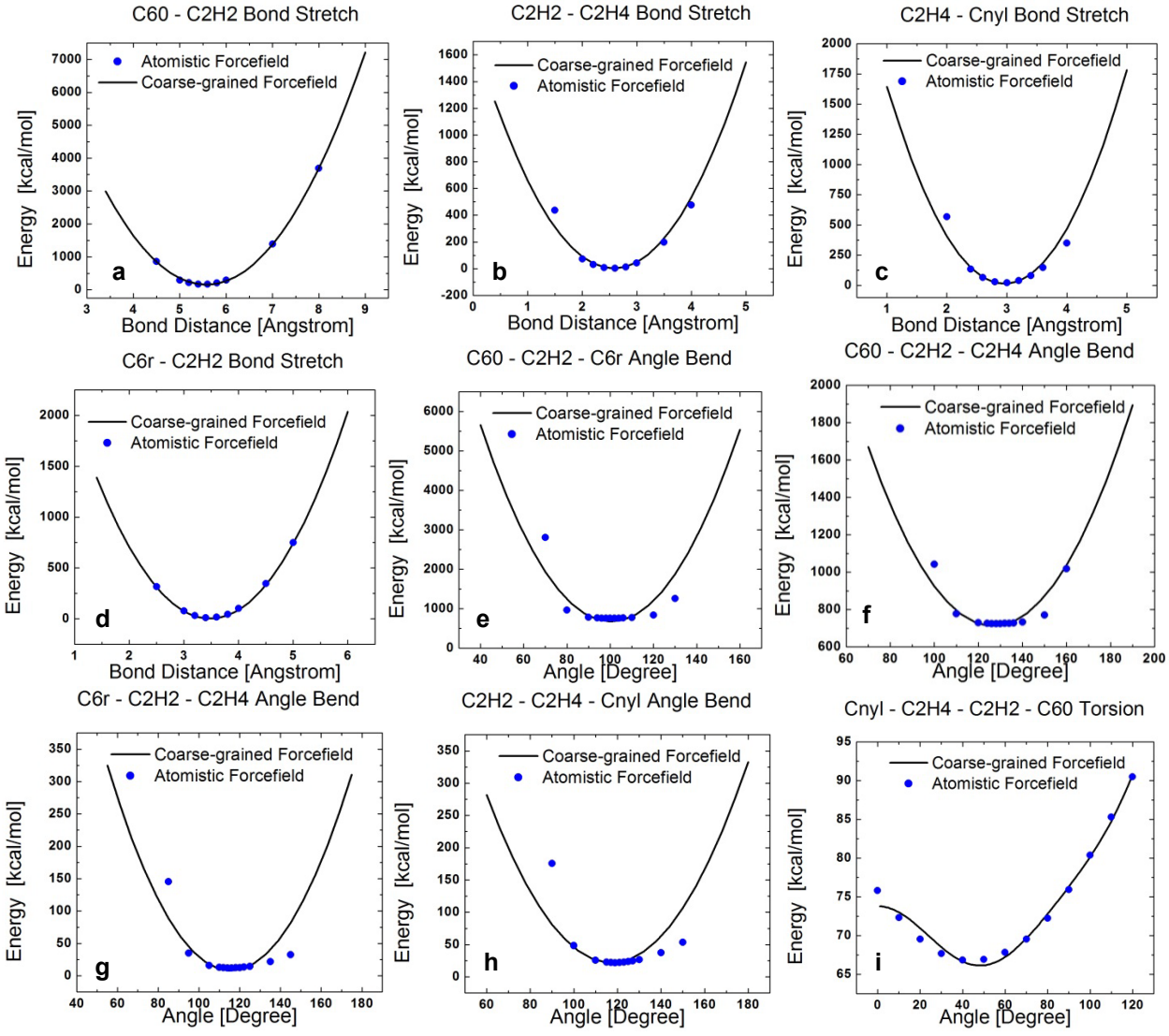

Figure. B2. Fitting against atomistic forcefield was used to obtain short range interaction parameters for coarse-grained forcefield. Here fitting results for all interaction contributions are shown with bond stretching terms: a) C60-C2H2, b) C2H2-C2H4, c) C2H4-Cnyl and d) C6r-C2H2; angle bending terms: e) C60-C2H2-C6r, f) C60-C2H2-C2H4 g) C6r-C2H2-C2H4 and h) C2H2-C2H4-Cnyl; and torsion term: i) Cnyl-C2H4-C2H2-C60

C. Energy Convergence of Different P3HT:PCBM Interface Configurations

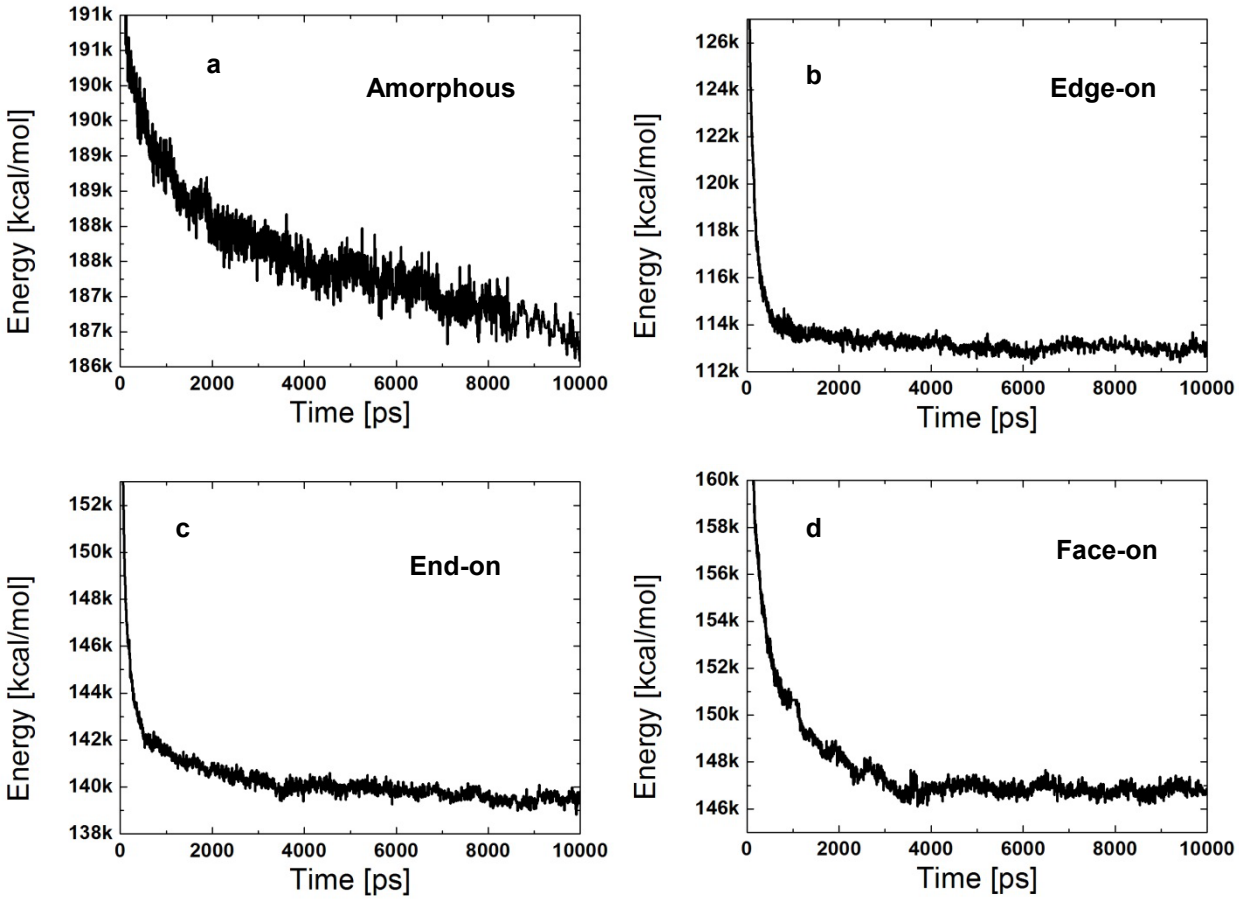

Figure. C1. Energy profile of different P3HT:PCBM interfacial configurations a) Amorphous, b) Edge-on, c) End-on and d) Face-on as a function of simulation time. It is clear that for interfaces between crystalline P3HT and PCBM (b-d), convergence is achieved after about 4,000 ps. For amorphous P3HT:PCBM interface (a) a linear reduction of system energy is observed after 10,000 ps which is attributed to the more pronounced intercalation of PCBM into amorphous P3HT. Analysis of the amorphous P3HT:PCBM interface at a much later time frame would have to be carried out over a more diffuse interface which reduces the accuracy of both interfacial energy calculation and PCBM intercalation analysis.