[Supplementary materials]

Atomistically informed hierarchical modeling for revisiting the constituent structures from heredity and nano-micro mechanics of sheath-core carbon fiber

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1. Complete intermediate variables parameters for the energy-matching bond stretching force fields

Table S1 - Calibrated Parameters for Morse-type and harmonic-type bond stretching terms

Bond type	Cluster model	$E_{el,\ cl}$ /(kcal/mol)	ν_e /(cm^{-1})	$\underline{r_e}$ /Å	$E_{el,fr1}$ /(kcal/mol)	$E_{el,fr2}$ /(kcal/mol)	$\underline{D_e}$ /(kcal/mol)	D_v /(cm^{-1})	M $/(g/mol)$	α /(Å^{-1})	$\underline{K}$ (kcal/mol•Å^2)
C^{ring}_C^{ring}	C_6H_6	-1.45551*10^5	1510.44	1.398	$C_6H_6^{(3)}$ -1.45397*10^5	/	152.71	5.34*10^4	6	1.964	589.03
C^{ring}_N^{ring}	C_5H_5N	-1.55602*10^5	1511	1.335	$C_5H_5N^{(3)}$ -1.55478*10^5	/	123.37	4.34*10^4	6.462	2.268	634.85
C^{sp3}_C^{sp3}	C_2H_6	-5.0020*10^4	1415.48	1.528	$CH_3^{(2)}$ -2.4961*10^4	$CH_3^{(2)}$ -2.4961*10^4	98.58	3.45*10^4	6	2.291	517.41
C^{sp2}_O^{sp2}	HC(O)H	-7.1761*10^4	1862.96	1.200	$CH_2^{(3)}$ -2.4532*10^4	$O^{(3)}$ -4.7045*10^4	183.70	6.43*10^4	6.857	2.361	1024.04
C^{sp3}_H	CH_4	-2.5385*10^4	3019.05	1.100	$CH_3^{(2)}$ -2.4961*10^4	$H^{(2)}$ -312.41	112.28	3.93*10^4	0.923	1.796	362.01
C^{ring}_N^{sp3}	$C_6H_5NH_2$	-1.80245*10^5	1342.22	1.374	$C_6H_5^{(2)}$ -1.45120*10^5	$NH_2^{(2)}$ -3.5014*10^4	111.66	3.91*10^4	6.462	2.118	500.95
C^{ring}_O^{sp3}	C_6H_5OH	-1.92700*10^5	1314.07	1.359	$C_6H_5^{(2)}$ -1.45120*10^5	$OH^{(2)}$ -4.7461*10^4	118.50	4.15*10^4	6.857	2.074	509.51
C^{sp}_C^{sp3}	CH_3CN	-8.3194*10^4	1388.59	1.459	$CH_3^{(2)}$ -2.4961*10^4	$CN^{(2)}$ -5.8102*10^4	131.59	4.60*10^4	6	1.945	497.83
C^{ring}_H	C_6H_6	-1.45551*10^5	3166.61	1.093	$C_6H_5^{(2)}$ -1.45120*10^5	$H^{(2)}$ -312.41	118.34	4.14*10^4	0.923	1.835	398.26
C^{sp}_N^{sp}	HCN	-5.8547*10^4	2216.25	1.155	$CH^{(4)}$ -2.4094*10^4	$N^{(4)}$ -3.4207*10^4	247.28	8.65*10^4	6.462	2.350	1365.78
N^{sp3}_H	NH_3	-3.5438*10^4	3440.8	1.023	$NH_2^{(2)}$ -3.5014*10^4	$H^{(2)}$ -312.41	111.90	3.92*10^4	0.933	2.061	475.31
O^{sp3}_H	CH_3OH	-7.2521*10^4	3822.87	0.965	$CH_3O^{(2)}$ -7.2101*10^4	$H^{(2)}$ -312.41	107.27	3.75*10^4	0.941	2.349	591.76
C^{ring}_C^{sp3}	$C_6H_5CH_3$	-1.70189*10^5	1456.53	1.508	$C_6H_5^{(2)}$ -1.45120*10^5	$CH_3^{(2)}$ -2.4961*10^4	108.79	3.81*10^4	6	2.244	547.73
C^{sp3}_O^{sp3}	CH_3OH	-7.2521*10^4	1070.19	1.407	$CH_3^{(2)}$ -2.4961*10^4	$OH^{(2)}$ -4.7461*10^4	98.82	3.46*10^4	6.857	1.849	337.93
C^{sp3}_N^{sp3}	CH_3NH_2	-6.0067*10^4	1082.97	1.457	$CH_3^{(2)}$ -2.4961*10^4	$NH_2^{(2)}$ -3.5014*10^4	92.68	3.24*10^4	6.462	1.876	326.12

Multiplicity values are labeled in parentheses and key variables are marked with underlines.

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2. Intermediate variables and interpolation configurations of the proposed bond stretching potential

Table S2 – Critical distance parameters and interpolation step length configurations (ISLC)

Bond Type	$r_{critical/Å}$	**Bond Type**	$r_{critical/Å}$
C^{ring}-C^{ring}	1.6116	C^{ring}-H	1.3327
C^{ring}-N^{ring}	1.5216	C^{sp}-N^{sp}	1.3115
C^{sp3}-C^{sp3}	1.6917	N^{sp3}-H	1.2197
C^{sp2}-O^{sp2}	1.3553	O^{sp3}-H	1.1217
C^{sp3}-H	1.3484	C^{ring}-C^{sp3}	1.6778
C^{ring}-N^{sp3}	1.5617	C^{sp3}-O^{sp3}	1.6435
C^{ring}-O^{sp3}	1.5537	C^{sp3}-N^{sp3}	1.6879
C^{sp}-C^{sp3}	1.6762		

ISLC for the bond stretching energy and force terms

$$\Delta r = \begin{cases} 0.01 r_{critical} & r \le r_{critical} \\ 0.01\left(r_c - r_{critical}\right) & r_{critical} < r \le r_c \end{cases}$$

3. The remaining parameters of the force fields

Table S3 – Unlisted parameters of the dihedral, improper torsion, van der Waals potentials and special bonds weighing coefficients

Dihedral central atoms	K_d /(kcal/mol)	d	n	Improper central atoms	K_i /(kcal/mol)	ω_0 /°
C^{sp3} - C^{sp3}	1	1	3	C^{ring} - C^{ring}	20	0
C^{sp3} - C^{ring}	1	1	3	C^{sp3} - C^{ring}	20	0
C^{ring} - C^{ring}	12.5	-1	2	C^{ring} - N^{ring}	20	0
C^{ring} - N^{ring}	12.5	-1	2			
C^{sp} - C^{sp3}	0	1	1			
C^{ring} – N^{sp3}	1	1	3			
C^{ring} – O^{sp3}	1	-1	2			

vdW atom pairs	$\epsilon/(kcal/mol)$	σ/Å	vdW atom pairs	$\epsilon/(kcal/mol)$	σ/Å
C^{ring}-C^{ring}	0.064	4.01	O^{sp2}-O^{sp2}	0.267	3.3
N^{sp2}-N^{sp2}	0.041	3.57	O^{sp3}-O^{sp3}	0.267	3.535
C^{sp3}-C^{sp3}	0.054	4.01	C^{sp}-C^{sp}	0.064	4.01
H-H (bounded to C)	0.02	2.995	N^{sp3}-N^{sp3}	0.106	4.07
N^{sp}-N^{sp}	0.065	3.57	H-H (bounded to O)	0.013	1.11

vdW 6th power mixing rules	$\epsilon_{ij} = \frac{2\sqrt{\epsilon_i \epsilon_j}\sigma_i^3 \sigma_j^3}{\sigma_i^6 + \sigma_j^6}$	$\sigma_{ij} = \left(\frac{1}{2}\left(\sigma_i^6 + \sigma_j^6\right)\right)^{\frac{1}{6}}$

Special bonds settings	1-2 weighing coefficients	1-3 weighing coefficients	1-4 weighing coefficients
	0	0	1

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4. Anharmonic bond stretching forces and energy perturbations calculated at the cutoff distance

Table S4 – Force and energy at the cutoff radius for each single bond

Bond Type	Force at the cutoff radius/(kcal/mol·Å)	Maximum attractive Force/(kcal/mol·Å)	Energy at the cutoff radius/(kcal/mol)	Equilibrium state energy/(kcal/mol)
C^{ring}_C^{ring}	-0.00131	-251.66	-0.000327	-152.71
C^{ring}_N^{ring}	-0.000767	-211.51	-0.000192	-123.37
C^{sp3}_C^{sp3}	-0.00121	-169.42	-0.000303	-98.58
C^{sp2}_O^{sp2}	-0.000593	-318.02	-0.000148	-183.7
C^{sp3}_H	-0.000326	-179.87	-0.0000816	-112.28
C^{ring}_N^{sp3}	-0.000800	-188.03	-0.000200	-111.66
C^{ring}_O^{sp3}	-0.000818	-198.38	-0.000204	-118.5
C^{sp}_C^{sp3}	-0.00146	-216.22	-0.000364	-131.59
C^{ring}_ H	-0.000325	-190.92	-0.0000813	-118.34
C^{sp}_N^{sp}	-0.000669	-427.62	-0.000167	-247.28
N^{sp3}_H	-0.000203	-187.01	-0.0000507	-111.9
O^{sp3}_H	-0.000136	-185.47	-0.0000340	-107.27
C^{ring}_C^{sp3}	-0.00126	-186.00	-0.000315	-108.79
C^{sp3}_O^{sp3}	-0.000944	-159.84	-0.000236	-98.82
C^{sp3}_N^{sp3}	-0.00106	-150.59	-0.000265	-92.68

the negative sign represents the attractive force or energy

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