

Structural Dynamics of Carbon Dots in Water and N,N-Dimethylformamide Probed by All-Atom Molecular Dynamics Simulations

*Markéta Paloncýová, Michal Langer, Michal Otyepka**

Regional Centre of Advanced Technologies and Materials, Department of Physical
Chemistry, Faculty of Science, Palacky University in Olomouc, 17. listopadu 1192/12, 771 46
Olomouc, Czech Republic

Installation Instruction for VMD Carbon Dot Builder:

- Download CD builder on <http://cd-builder.upol.cz>
- Install VMD 1.9.3 or later
- In VMD directory go to `plugins/noarch/tcl`
- Replace `Nanotube1.5` directory with the provided one
- In case of issues see the web page or REAMDE file

VMD Builder

Based on experimental observations of CDs,¹ the builder uses a hexagonal graphene-like sheet as a basic shape, for which the user can set the edge size in units of number of benzene rings (`#BR`). Here, we will first describe the basic pattern and afterwards the handling of the edges. In the description, we used j as the carbon line number (starting from 0, see Figure S1), i as the cell number in a line, a as the bond length and `#BR` as the preset number of benzene rings on the layer edge.

As an unit cell, the builder uses two atoms of a benzene ring (see Figure S1, opaque red and green dot), where each atom is defined by a vector ($r1=[0,0,0]$ and $r2=[a*\sin60^\circ, -a*\cos60^\circ, 0]$, respectively) from the cell position. Initially, the cell repeats (`#BR+1+j`) times until the end of line j with the x -repeating distance $Lx=2a*\sin60^\circ$ (cell positions are depicted as transparent red dots in Figure S1). The next line j starts with y -repeating distance

$Ly = a + a \cos 60^\circ$ and is shifted in x by $-j \cdot a \sin 60^\circ$. This continues #BR-times until the middle of a layer and then the number of cells is reduced every line by 1 until $j = \#BR \cdot 2 - 1$. The last cells in the lines, where $j < \#BR$ are represented by just a $r1$ atom. The first cells in lines where $j > \#BR$, are represented by just a $r2$ atom.

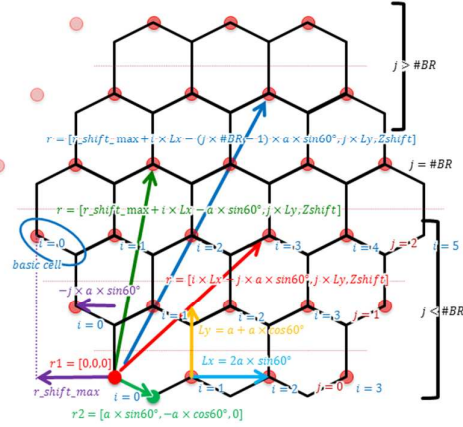


Figure S1: Schematic of the CD building script. The unit cell i is represented by two atoms (full non-transparent red and green circles) defined by vectors from the unit cell positions (red circles). In each line j , the position of an unit cell moves by Lx and the next line is shifted along the y -axis by Ly . Differences originating from the hexagonal shape of a layer are displayed in three classes, $j < \#BR$ (number of benzene rings, here equals 3), $j = \#BR$ and $j > \#BR$ and in each group the positions of basic cells are defined by the r vector.

Surface functional groups of CDs (either hydrogens or oxygen-containing functional groups on the edges) were added according to a vector from a bound atom (Figure S2). Although the builder works initially with vectors starting from the unit cell positions, the edge vectors need to be set from the surface bound atoms in order to properly rotate the functional groups with a larger number of atoms (e.g., carboxyl). Six different edges and correspondingly six different vectors are defined using the already introduced cell number i , line number j and number of benzene rings $\#BR$. A schematic of the edge vectors can be seen in Figure S2. Each of the surface functional groups is defined separately: each of the atoms is described by a bond length and angle with respect to the edge vector and $[0,0,0]$, which is the position of an atom bound to the CD hexagonal sheet. When the group is placed on a desired edge position, it is rotated. Therefore, the first atom outside of the benzene rings lies on the edge vector and the others face the outer environment with internal angles as defined initially for the group. The geometry of the groups is displayed in Figure S3. With this approach, other surface functional groups can be easily added in the future. For the sake of easier manipulation with the structures (see later), we added all groups into the layer plane. The built dot therefore needs to be properly minimized.

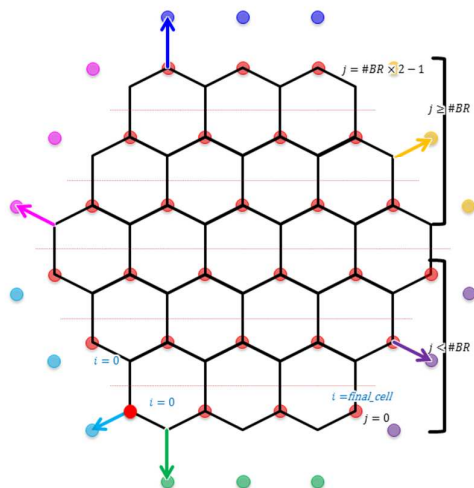


Figure S2: Edge vectors defining the direction of surface groups on each of the six edges (denoted by different colors).

After building a whole layer, another layer is started above it separated by 0.335 nm. The number of benzene rings on each edge stays the same for the second layer but then is reduced by one until the number of layers defined by the user is reached. In principle, instead of a spherical dot, the user can define just a few large layers for a graphene dot. The starting point for layer building is shifted to preserve the spherical geometry and AB stacking. This shift is $[k*3/2*a*\sin60^\circ - 2*a*\sin60^\circ]$ along the x axis and $[k/2*(4*a+a*\cos60^\circ-2*a)]$ along the y axis (where k is the number of layers starting from 0 for the middle layer) for the even layers, whereas the odd layers are shifted by $[(k-1)/2*3*a*\sin60^\circ-a*\sin60^\circ]$ along the x axis and $[-a+a*\cos60^\circ+((k-1)/2)*(4*a+a*\cos60^\circ)]$ along the y axis. The number of layers above the middle layer is specified by the user in the GUI (Figure S4). After the ‘upper part’ of the dot (z axis coordinates ≥ 0) has been completed, the lower part is built in a similar way, decreasing the z coordinate every layer by 0.335 nm, starting from the second layer.

By default, the dangling bonds on the edges of each layer are saturated with hydrogens. However, CDs usually contain significant amounts of, e.g., oxygen or nitrogen bearing functional groups. Therefore, edge functional groups can be added. In the present study, we considered hydroxyl, carbonyl and carboxyl (in both deprotonated/charged and protonated/uncharged forms) groups (see Figure S3). The geometry of hydroxyls and carboxyls had to be slightly modified to allow artificially assigned bonds between close groups (both are a bit stretched from the layer edge). The structure relaxes during the energy minimization. The user can choose whether the groups reside on neighboring benzene rings or not (if not, the surface coverage can only reach $\sim 50\%$). At each position, addition of the group is decided based on a randomly chosen number (0-1) – if it falls within the interval of the fraction of dot coverage, the functional group is added, if not, hydrogen is added. The fraction of surface coverage then corresponds on average to the desired value, but with the same setup, different CDs can be created.

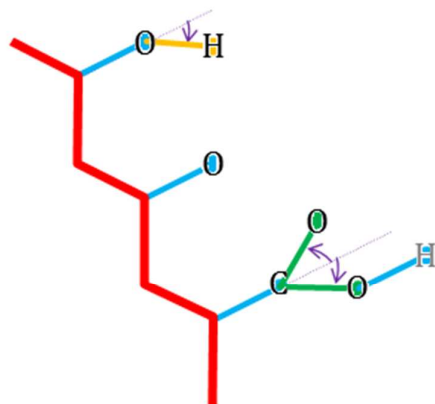


Figure S3: Surface functional group geometry: each atom is defined by vectors and/or an angle. The red line represents the edge of a CD sheet. The blue lines correspond to the edge vector defined for each CD edge (see Figure S2). The violet arrows represent 30° . The orange line is a bond of length 1.4 nm, whereas the green line is a longer bond by 30 %. The hydrogen in the carboxyl group can either be present (uncharged carboxyl) or missing (charged carboxyl). The geometry of the functional groups does not ideally reflect the true relaxed geometry (e.g., angles in hydroxyl or carboxyl groups) but allows assignment of proper bonds with the expectation of following structure relaxation.

Another possibility for handling the edge functional groups is by manual addition. The user can use this approach either for a pure CD covered with hydrogens or for a prepared dot by the previously proposed random scheme. The user can change an edge hydrogen to a chosen functional group by clicking on it, or oppositely, the user can delete the atoms of an automatically added group and replace them with either hydrogen or another group. In this way, a CD with a mixture of functional groups can be prepared with any composition. Future development may focus on enabling doping of the CD core. Using the functionalities of Topotools,² it is also possible to save both the structure and GROMACS topology, i.e., a ‘fake’ one that requires atom type and charge adjustment (see later). These utilities were implemented in the CD VMD builder (<http://cd-builder.upol.cz>), which was built upon the graphene and nanotube builder³ already implemented in VMD 1.9.3.⁴

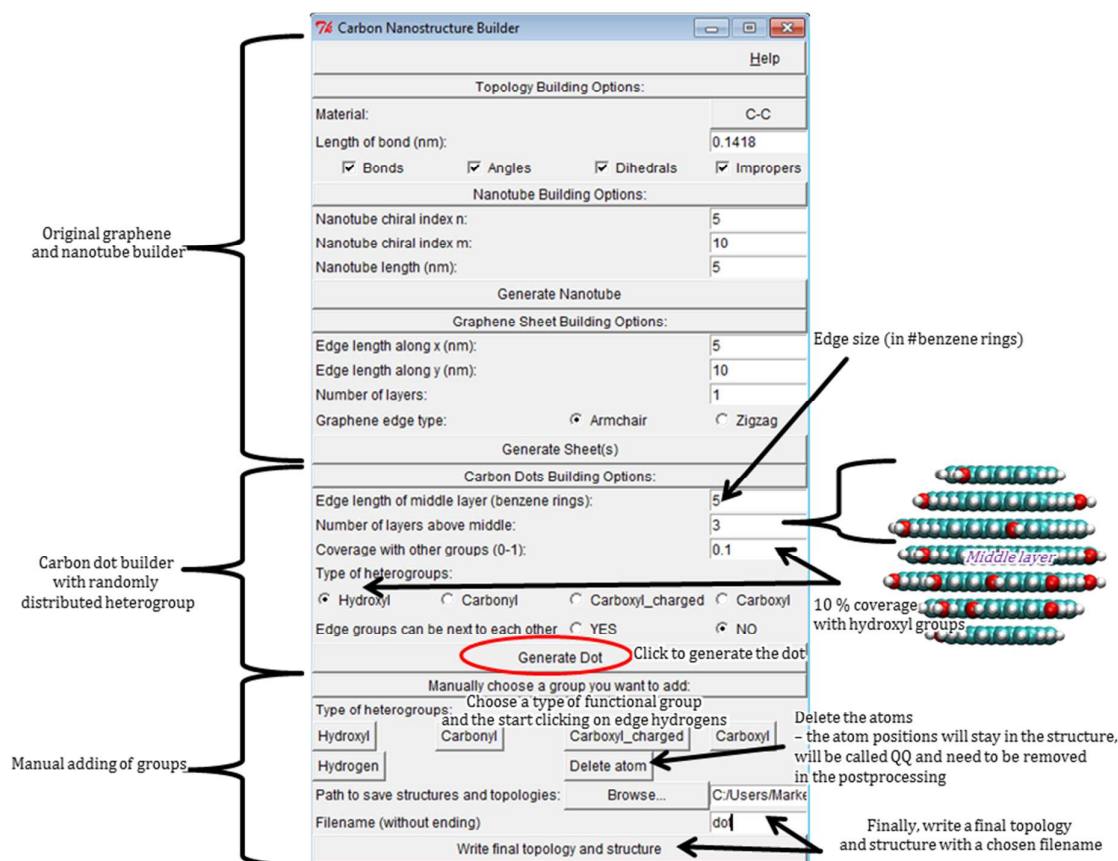


Figure S4: VMD carbon dot builder GUI

Charges and Force Field

For assigning the partial charges, we used circumcoronene and coronene models as they were small enough to allow quantum-chemical calculation and simultaneously large enough to act as polycyclic aromatic systems. First, all (functionalized, see later) circumcoronene molecules were fully optimized using the Becke three-parameter hybrid density functional B3LYP and 6-31++G(d,p) basis set as we used earlier.⁵ Assignment of the partial charges on individual atoms was based on fitting the electrostatic potential calculated on different coronene and circumcoronene models using the CHELPG⁶ approach at the HF/aug-cc-pVDZ and HF/cc-pVDZ levels of theory in vacuum, respectively. Further, we calculated partial charges at the HF/6-31G* level of theory owing to its compatibility with the AMBER99 force field for subsequent simulations of the interaction of carbon dots with biomacromolecules. To obtain parameters compatible with the AMBER03 force field, we also calculated the partial charges in a solvent environment of dielectric constant $\epsilon_r = 4.0$ at the B3LYP/cc-pVTZ level of theory on coronenes. All obtained sets of partial charges are summarized in Tables 1 and the S1.

The electrostatic potential derived partial charges calculated in the core of the layers were negligible, and hence taking into account the homogeneity of the region and possible simplicity, we considered them to be zero. For each of the functional groups, we prepared several circumcoronene molecules with various positions and amount of functional groups.

These were further sorted according to their position (in zig-zag or armchair conformation) and the partial charges assigned to the atoms of various types (see e.g., Figure S5) were averaged. We observed significant differences on zig-zag and armchair edges in both the surface group atoms and edge aromatic carbons (the smaller coronene model used as a first guess did not contain zig-zag edges, and therefore we switched to using the larger circumcoronene). We also analyzed the atom charges on atoms not connected directly to the oxygen-containing functional groups (e.g., lying on a neighboring ring, etc.) and observed two common differences for a carbon in the same benzene ring as the functional group ('nearby carbon', for atom type assignment, see Figure S5) and a carbon on a neighboring benzene ring ('next-ring carbon'). Both were found already in the coronene models (armchair). The changes in the charge of a nearby carbon in the zig-zag conformation were small, and thus for simplicity, we treated these carbons as 'ordinary carbons'.

Although initially we performed simulations with partial charges calculated on coronene models only (Figure S7, resulting MD simulations not shown), the observed trends in CD behavior did not differ significantly from the results presented here, and therefore the model was deemed robust enough to handle small uncertainties in charges. Generally, the differences in the partial charges calculated on the smaller system (coronene) were not significant; the functional groups were just slightly more polarized. We also analyzed the effect of changing the number of functional groups on coronene based models and observed very little dependency of the partial charge on the total number of functional groups in most of the cases. For hydroxyls, we considered several coronene models with two hydroxyls on the same ring differing in their mutual positions and found that the charge on the carbon atoms binding the hydroxyls was significantly affected by the nearby functional group. In the case of charged carboxyls, the polarity of the functional group increased with the total number of carboxyls on coronene and the individual partial charges differed by up to 0.1 e. The partial charges of CD models immersed in a dielectric with $\epsilon_r = 4.0$ were slightly reduced as expected. In most cases, the differences were small, but in the case of charged carboxyl groups, we observed differences of up to 25 % in the resulting charge. For simulations of more complex systems, we advise that partial charges most compatible with the chosen force field are used for other compartments of the complex system. Generally, we recommend that the usage and parameterization of partial charges should be considered carefully by the user for each specific case because in a conjugated system, a local change of chemistry can cause a distant change in the electrostatic potential and calculated partial charges.

In the presented approach we calculated the average charges of individual atom types and assign them to the structure of each built CD layer (Table S1 and Figure S6). Further, we used the next layer of carbons (not attached to any surface groups, 'neutralization layer' in Figure S7) for charge neutralization of that CD layer (naturally except for the case of charged carboxyl groups where the total charge is negative). Nevertheless, we observed some minor residual charges stemming from the numerical residues in the distribution of charges. Hence, we added these 'tiny' charges into another layer of carbons and the very last part was assigned to the first carbon in the topology. From our experience, this residual artificially assigned charge is so small that it only affects the third decimal place and does not play a significant role in the behavior of the resulting CD. Here in the Supporting Information, we detail the

nomenclature of the carbons in the layers and also the individual molecules with calculated partial charges used for the final charge estimations (Figure S7).

Bibliography

- (1) Holá, K.; Zhang, Y.; Wang, Y.; Giannelis, E. P.; Zbořil, R.; Rogach, A. L. *Nano Today* **2014**, 9 (5), 590–603.
- (2) Kohlmeyer, A. 2017.
- (3) Robert R. Johnson; Kohlmeyer, A. .
- (4) Humphrey, W.; Dalke, A.; Schulten, K. *J. Molec. Graph.* **1996**, 14, 33–38.
- (5) Sudolská, M.; Dubecký, M.; Sarkar, S.; Reckmeier, C. J.; Zbořil, R.; Rogach, A. L.; Otyepka, M. *J. Phys. Chem. C* **2015**, 119 (23), 13369–13373.
- (6) Breneman, C. M.; Wiberg, K. B. *J. Comput. Chem.* **1990**, 11 (3), 361–373.
- (7) Cheng, A.; Steele, W. A. *J. Chem. Phys.* **1990**, 92 (6), 3858.

Table S1: Atomic properties showing for each functional group the atom names assigned by the VMD builder, atom types used in the topology (CA atoms in each groups are edge carbon atoms connected to the functional group) and the charges on the atoms calculated initially on coronene models (for hydroxyl groups we had models also with two hydroxyls on a same group, in brackets we provide averages for models with maximum one hydroxyl on ring), in diethylether ($\epsilon = 4$) for AMBER03 and by HF/6-31G* for AMBER99SB on circumcoronene models in armchair and zig-zag conformations.

Group /Atom	VMD name	Atom types		Atom charge				Near-by carbon	Next-ring carbon
		OPLS-AA	AMBER99SB	HF/aug-cc-pVTZ	B3LYP/cc-pVTZ	HF/6-31G*			
				Vacuum	$\epsilon = 4$	Armchair	Zig-zag		
				Armchair (coronene)		(circumcoronene)			
Edge C	CA	Cheng&Steele ⁷	Cheng&Steele ⁷ (CS)	-0.210					
Edge H	HA	OPLS 146	HA	0.179					
Pure CD	CA	Cheng&Steele ⁷	Cheng&Steele ⁷ (CS)	-0.210	-0.230	-0.180	0.400		
H	HA	OPLS 146	HA	0.130	0.150	0.115	0.180		
Hydroxyl	CA	OPLS 166	Cheng&Steele ⁷ (CS)	0.279 (0.354)	0.252	0.337	0.218	-0.452	-0.292
O	OH	OPLS 167	OH	-0.578 (-0.583)	-0.557	-0.647	-0.590		
H	HO	OPLS 168	HO	0.415 (0.405)	0.435	0.443	0.430		
Carbonyl	CA	OPLS 320	C	0.69	0.526	0.705	0.560	-0.371	-0.27
O	ON	OPLS 340	O	-0.57	-0.464	-0.580	-0.540		
Carboxyl (0)	CA	Cheng&Steele ⁷	Cheng&Steele ⁷ (CS)	-0.131	-0.056	-0.117	-0.378	-0.223	-0.214
C	CX	OPLS 267	C	0.813	0.649	0.773	0.913		
O	OX	OPLS 269	OH	-0.635	-0.553	-0.600	-0.648		
O	OC	OPLS 268	O	-0.629	-0.554	-0.627	-0.655		
H	HX	OPLS 270	HO	0.428	0.425	0.440	0.440		
Carboxyl (-1)	CA	Cheng&Steele ⁷	Cheng&Steele ⁷ (CS)	-0.152	-0.032	-0.177	-0.323	-0.283	-0.231
C	CR	OPLS 271	C	1.045	0.726	0.980	1.093		
O	OR	OPLS 272	O2	-0.909	-0.778	-0.880	-0.906		
O	OK	OPLS 272	O2	-0.909	-0.778	-0.880	-0.906		

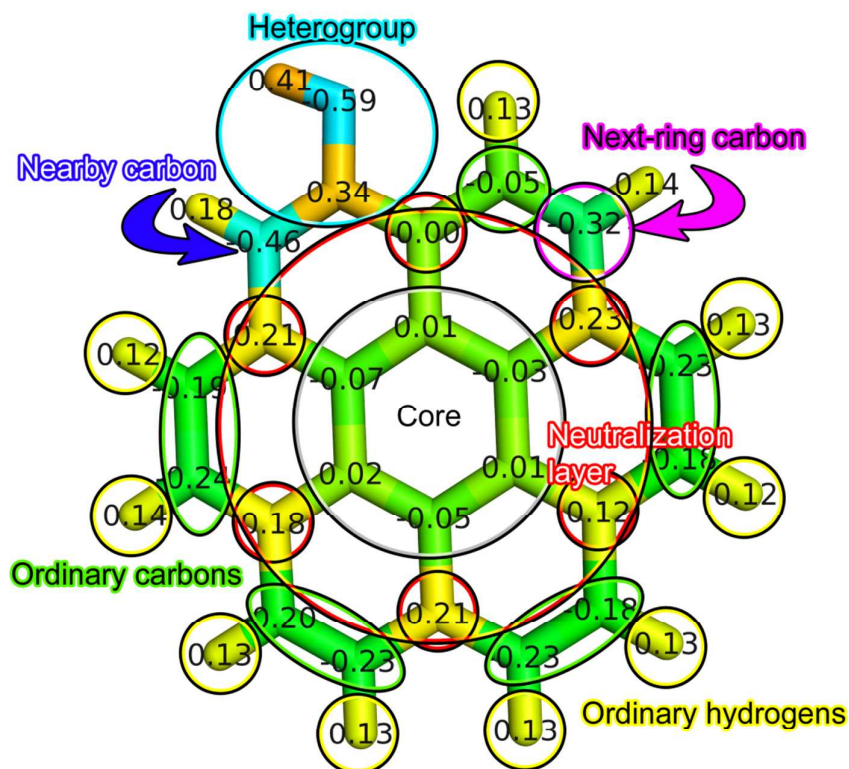


Figure S5: Nomenclature of the atoms in carbon dot layers as used for charge assignment in the text.

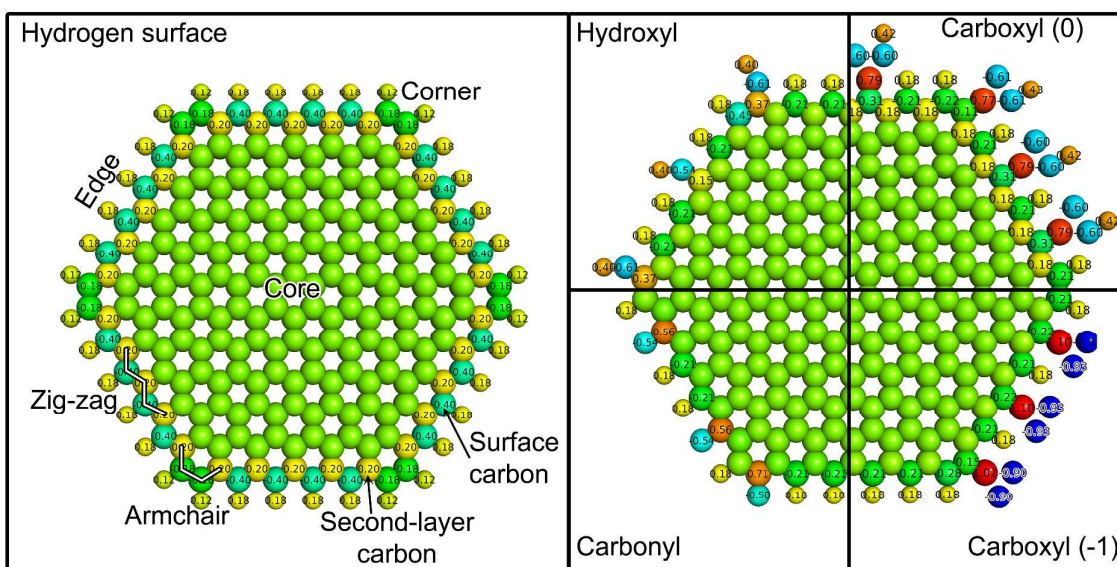


Figure S6: Charges assigned to atoms in CD layer without any surface modification (left, with noted nomenclature) and with hydroxyls, carbonyl, carboxyl, and deprotonated carboxyl on their edges (displayed quarters of individually simulated layers). We noted differences in charges for armchair and zig-zag conformations. Atoms in the layer core are with zero charges, second-layer carbons neutralize the layer.

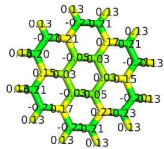
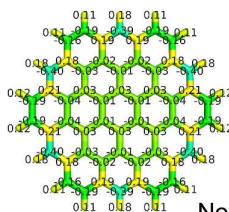
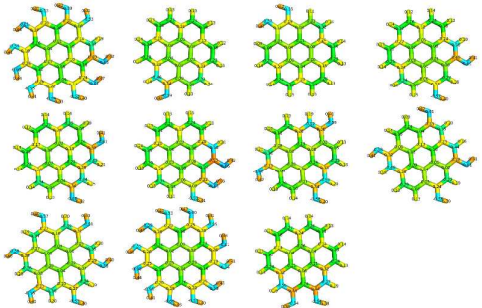
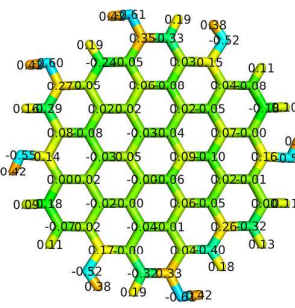
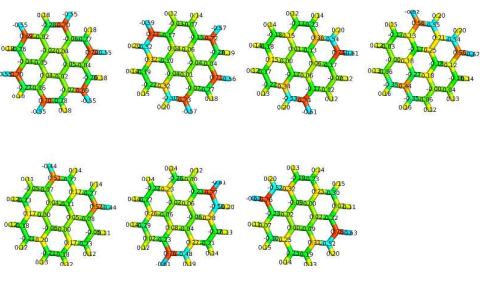
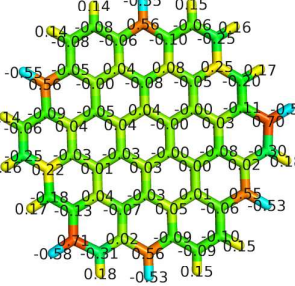
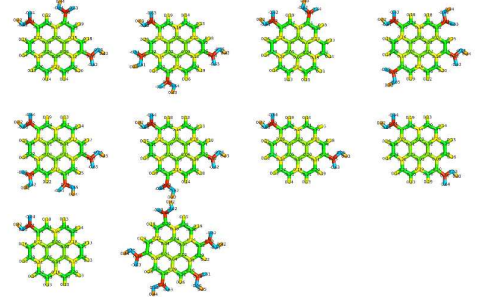
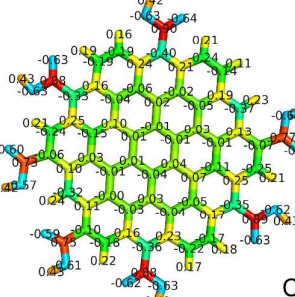
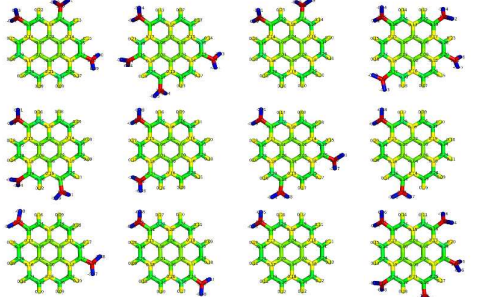
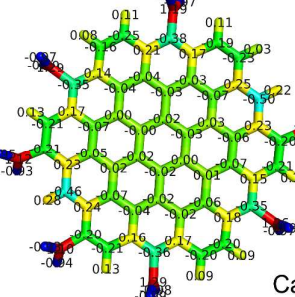
Coronene	Circumcoronene
	 No surface group
	 Hydroxyl
	 Carbonyl
	 Carboxyl (0)
	 Carboxyl (-1)

Figure S7: Partial charges calculated on different models of coronenes and circumcoronenes used for the estimation of molecular mechanics partial charges.

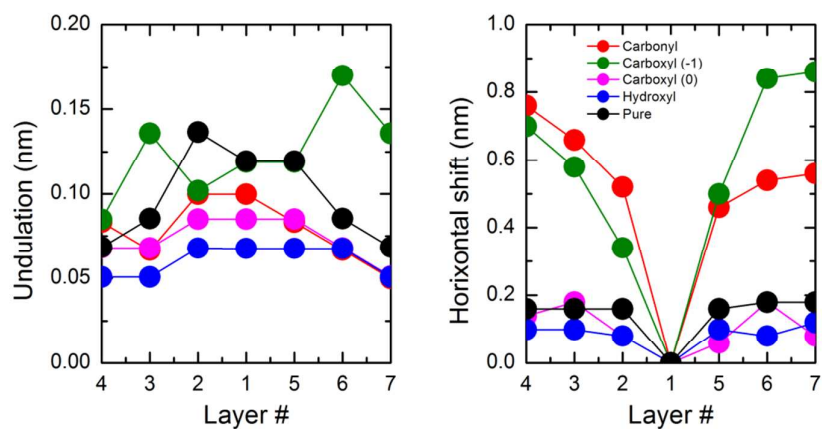
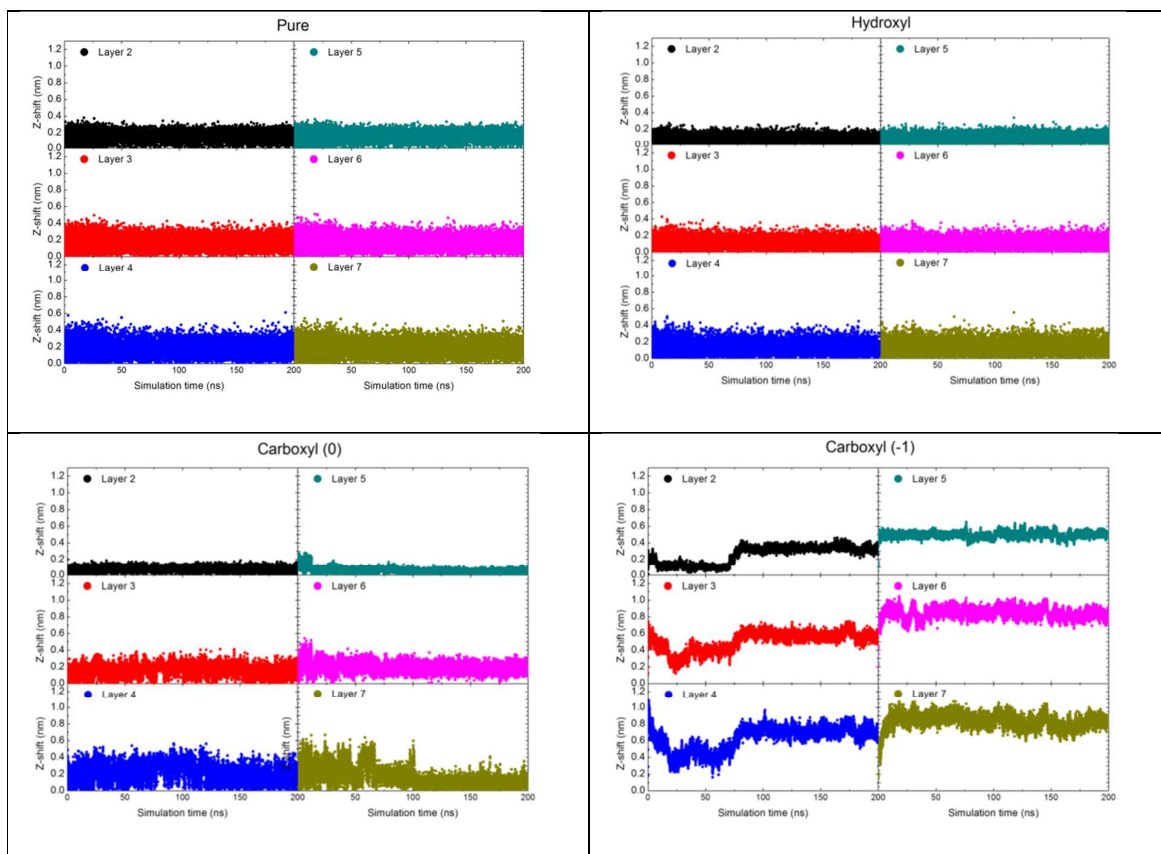


Figure S8: Layer undulation (width of density peak of individual layers) and their horizontal shifts from the middle layer. The middle layer is labeled as Layer 1.



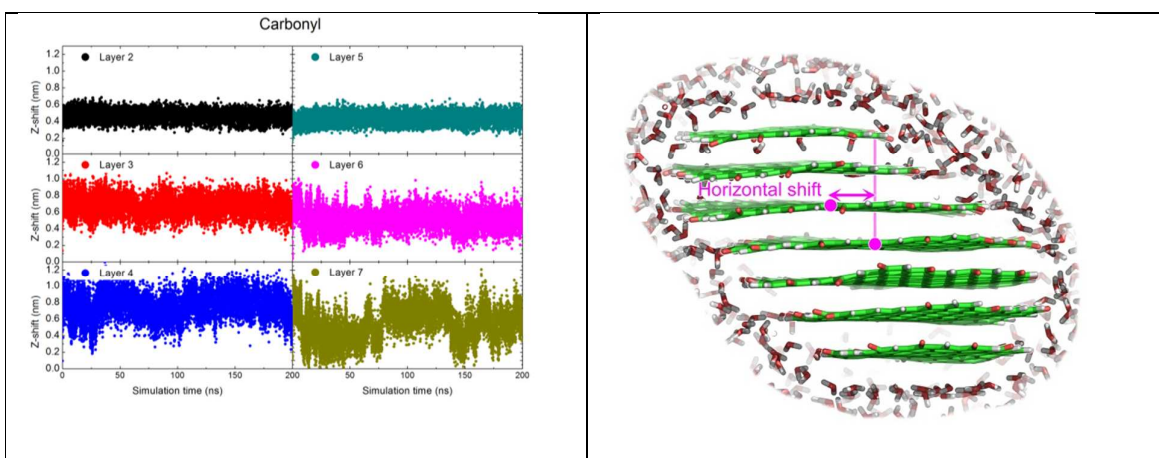


Figure S9: Horizontal shift (z-shift) of the individual layers in carbon dots during first 200 ns of simulations. Left and right columns in plots represent opposite semispheres of CD (Layer 2 and Layer 5 and next to the middle layer, Layers 4 and 7 are the furthest ones).

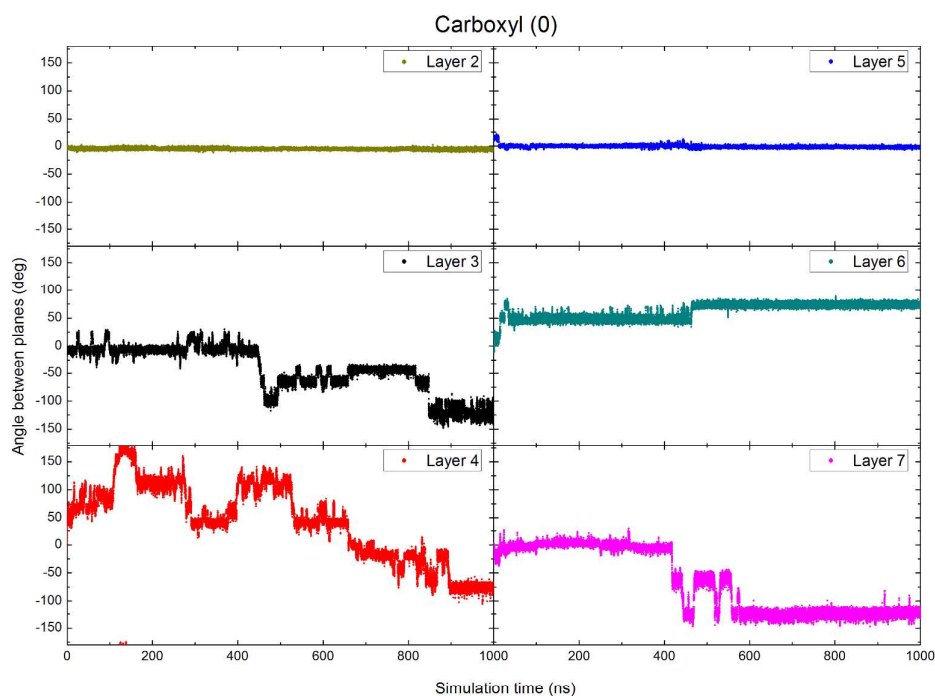


Figure S10: Orientation of the individual layers in respect to the neighboring layer during simulation of CD covered with uncharged carboxyls. The rotation increases with the distance from the middle layer (top to down in the plots).

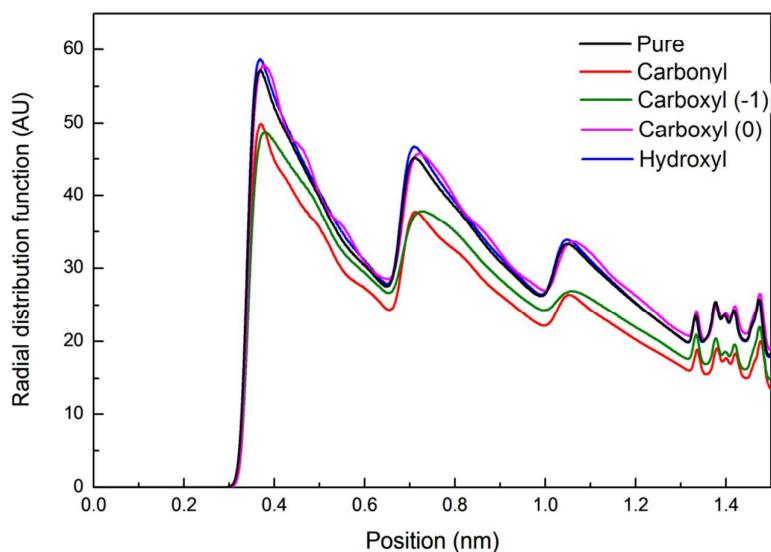


Figure S11: Radial distribution function of carbons around each other with exclusions of close bonded interactions (the small peaks at right side of the plot are caused by very far bonded interactions). The first peak corresponds to the position of carbons in AB stacking, other peaks are separated by 0.34 nm, corresponding to the layer spacing.

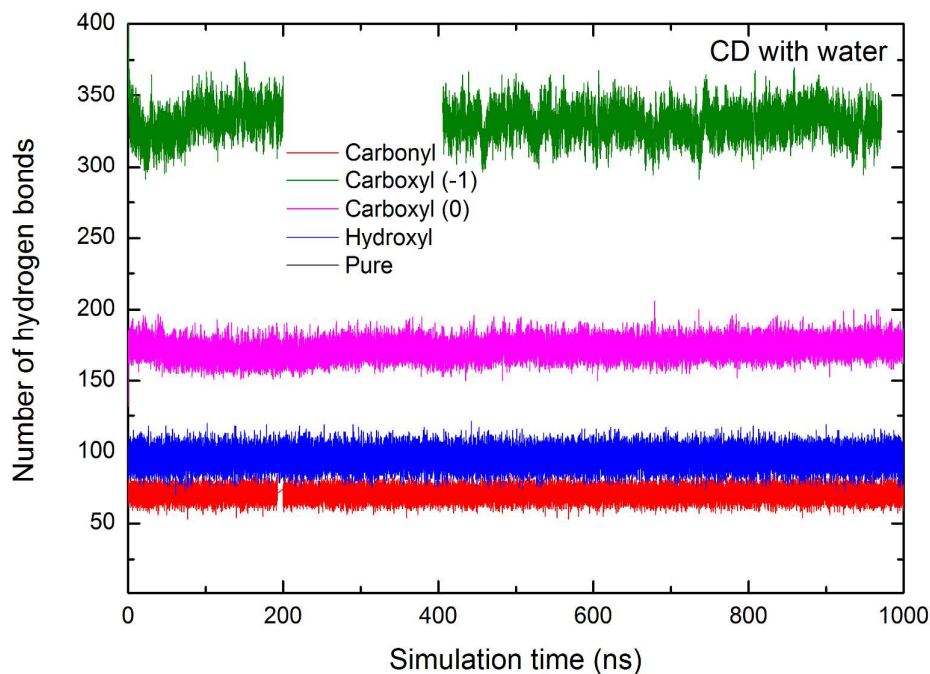


Figure S12: Number of hydrogen bonds between carbon dot and solvent (bottom). In charged carboxyls a period between 200 and 400 ns could not be displayed due to data loss.

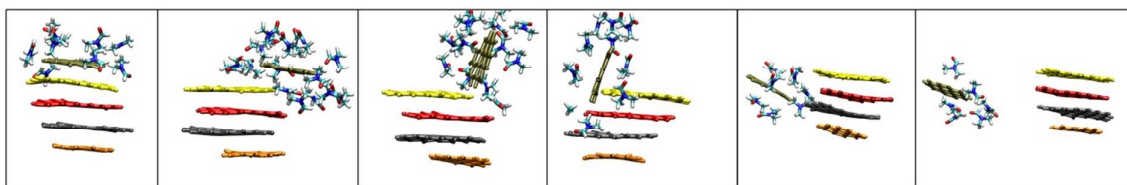


Figure S13: Sliding and separation of a coronene layer in dimethylformamide (DMF). Only DMF within 0.3 nm from the layer are displayed.

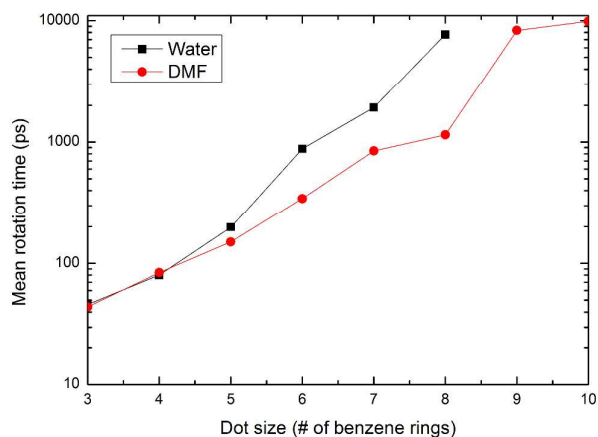


Figure S14: Mean time of two middle layers of a dot of certain size spent in a mutual conformation of $30 \pm k \cdot 60^\circ$ in the simulation.

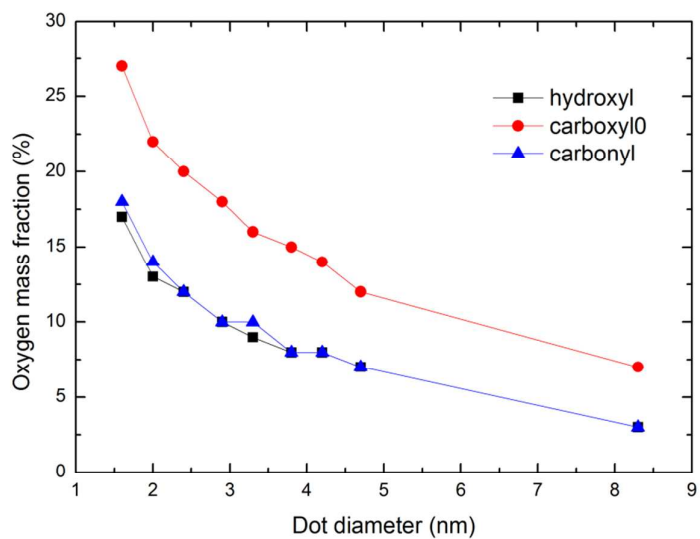


Figure S15: Mass fraction of oxygen in CDs with ~45% edge coverage.

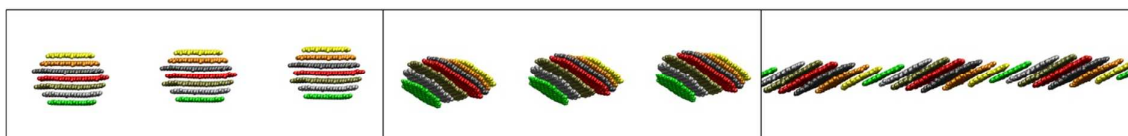


Figure S16: Carbonyl-covered carbon dot creating periodic particle. For clarity, no solvent is displayed. We show here three periodic images.

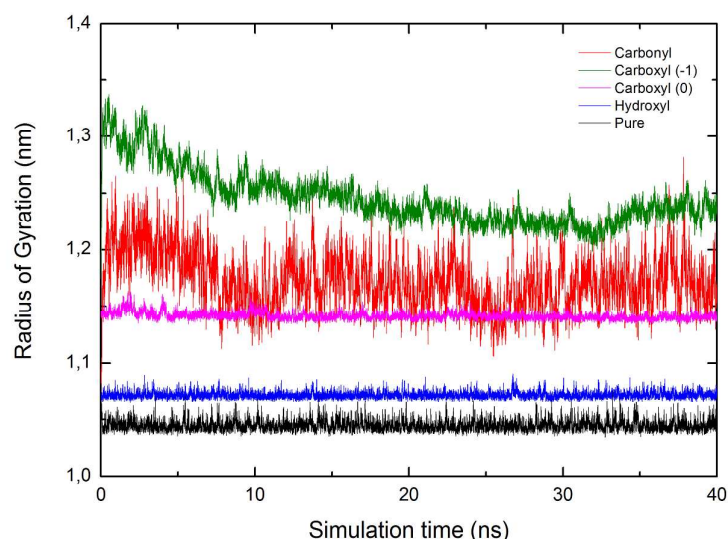


Figure S17: Gyration radii of CDs (six benzene rings on each edge, 30% coverage of functional groups or pure CD) studied during the equilibration stage of the simulations.

Table S2: Performed simulations and their lengths in ns. Yellow fields mean a simulation also in dimethylformamide (DMF).

Side size	Water																	DMF
(# of benzene rings)	Pure	Carbonyl			Hydroxyl			Carboxyl (0)			Carboxyl (1)							
Surface coverage (%)	0	10	30	50	10	30	50	10	30	50	1	2	3	5	10	30	50	0
3	50	50	50	50	50	50	50	50	50	50					50	50	50	50
4	50	50	50	50	50	50	50	50	50	50					50	50	50	50
5	50	50	50	50	50	50	50	50	50	50	50	50		50	50	50	50	50
6	1000	50	1000	50	50	1000	50	50	1000	50	50		50		50	1000	50	200
7	50	50	50	50	50	50	50	50	50	50					50	50	50	50
8	50	50	50	50	50	50	50	50	50	50					50	50	50	50
9	50	50	50	50	50	50	50	50	50	50					50	50	50	50
10	50	50	50	50	50	50	50	50	50	50	50				50	50	50	50
18	44	50	50	50	50	50	50	50	50	50					50	50	50	50

Table S3: Calculated properties of individual systems during the 50 ns simulations. The CD size is displayed in number of benzene rings. The data are colored according in a scale green-highest to red-lowest values.

		size	Carboxyl (-1)						Carboxyl (0)			Carbonyl			Hydroxyl			Pure				
			Water																			
Surface coverage			0.01	0.02	0.03	0.07	0.08	0.15	0.35	0.5	0.15	0.35	0.5	0.15	0.35	0.5	0.15	0.35	0.5	0	0	
Layer rotation time	ps	3						2066	16000	60	368	10158	nan	176	84	188	284	608	570	46	44	
		4						nan	nan	nan	2756	nan	nan	1070	332	422	838	17434	2120	80	84	
		5		366	652		3360	nan	nan	nan	nan	nan	nan	37926	3544	1402	6286	7270	4580	198	150	
		6	662	658		10976	nan	nan	nan	nan	nan	nan	nan	25148	5100	1132	5412	2884	26798	880	344	
		7						nan	nan	nan	nan	nan	nan	nan	4734	nan	6020	nan	9188	1914	846	
		8						nan	nan	nan	nan	nan	nan	nan	nan	5324	29722	nan	nan	7706	1144	
		9						nan	nan	nan	nan	nan	nan	nan	nan	nan	8352	nan	nan	nan	8324	
		10	nan					nan	nan	nan	nan	nan	nan	nan	nan	nan	nan	nan	nan	nan	9862	
		18						nan	nan	nan	nan	nan	nan	nan	nan	nan	nan	nan	nan	nan	nan	
Radius of gyration	nm	3						0.73	sep	sep	0.66	0.70	0.72	0.63	0.81	0.90	0.64	0.64	0.65	0.63	sep	
		4						0.84	0.91	sep	0.79	0.83	0.86	0.76	0.88	1.03	0.76	0.77	0.77	0.74	0.76	
		5		0.93	0.94		0.96	1.03	1.13	sep	0.96	1.02	1.07	0.93	1.02	1.28	0.93	0.94	0.95	0.87	0.93	
		6	1.06	1.06		1.09	1.13	1.25	sep	1.09	1.14	1.20	1.06	1.17	1.51	1.06	1.07	1.08	1.05	1.05		
		7						1.29	1.37	sep	1.27	1.32	1.37	1.23	1.32	1.68	1.24	1.25	1.25	1.18	1.18	
		8						1.42	1.55	1.62	1.40	1.47	1.49	1.37	1.44	1.99	1.37	1.38	1.39	1.35	1.35	
		9						1.59	1.69	1.87	1.56	1.73	1.67	1.53	1.61	2.02	1.50	1.55	1.56	1.48	1.52	
		10		1.67					1.71	1.85	2.09	1.70	1.75	1.79	1.67	1.74	2.12	1.67	1.68	1.69	1.65	1.66
		18						2.93	3.08	3.20	2.91	2.97	3.03	2.89	2.94	2.79	2.89	2.90	2.91	2.87	2.77	
Layer shift	nm	3						0.32	sep	sep	0.14	0.10	0.04	0.10	0.68	0.62	0.22	0.10	0.10	0.22	sep	
		4						0.30	0.40	sep	0.08	0.02	0.04	0.10	0.42	0.60	0.12	0.08	0.06	0.16	0.28	
		5		0.14	0.22		0.34	0.30	0.40	sep	0.08	0.08	0.26	0.12	0.28	0.54	0.12	0.08	0.08	0.16	0.28	
		6	0.16	0.22		0.32	0.36	0.14	sep	0.04	0.06	0.04	0.10	0.52	0.56	0.14	0.06	0.04	0.18	0.26		
		7						0.16	0.42	sep	0.10	0.06	0.20	0.06	0.44	0.54	0.12	0.04	0.04	0.16	0.14	
		8						0.32	0.38	0.30	0.06	0.30	0.04	0.06	0.26	0.56	0.08	0.06	0.04	0.16	0.10	
		9						0.30	0.52	0.76	0.06	0.60	0.24	0.06	0.26	0.42	0.08	0.06	0.04	0.16	0.08	
		10		0.14					0.08	0.48	0.58	0.06	0.06	0.24	0.08	0.28	0.44	0.10	0.06	0.06	0.12	0.06
		18						0.04	0.08	0.10	0.02	0.02	0.02	0.02	0.06	0.10	0.04	0.04	0.02	0.02	0.06	
Layer undulation	nm	3						0.15	0.12	0.24	0.07	0.09	0.09	0.19	0.17	0.15	0.10	0.10	0.06	0.07	0.26	
		4						0.11	0.18	0.13	0.10	0.10	0.10	0.08	0.15	0.10	0.15	0.09	0.10	0.10	0.31	
		5		0.18	0.13		0.13	0.12	0.14	0.16	0.12	0.10	0.13	0.11	0.11	0.14	0.11	0.11	0.09	0.12	0.32	
		6	0.11	0.11		0.10	0.12	0.16	0.23	0.15	0.16	0.14	0.12	0.10	0.16	0.11	0.10	0.10	0.13	0.28		
		7						0.13	0.29	0.29	0.12	0.15	0.23	0.11	0.16	0.14	0.13	0.11	0.13	0.11	0.30	
		8						0.15	0.23	0.36	0.13	0.32	0.25	0.13	0.15	0.17	0.12	0.11	0.11	0.12	0.21	
		9						0.15	0.19	0.36	0.15	0.42	0.33	0.14	0.18	0.20	0.12	0.11	0.10	0.15	0.25	
		10		0.14					0.15	0.21	0.46	0.17	0.24	0.44	0.15	0.19	0.20	0.15	0.11	0.11	0.15	0.26
		18						0.22	0.60	0.89	0.22	0.71	0.62	0.22	0.59	0.85	0.17	0.15	0.15	0.17	0.26	
Hydrogen bonds with solvent	#	3						68.4	121.6	170.4	36.0	61.8	76.5	18.3	33.7	39.1	18.6	37.1	45.3	nan	nan	
		4						91.5	171.8	228.0	50.8	93.1	113.3	24.6	38.8	44.9	26.5	49.1	64.8	nan	nan	
		5		24.1	36.0		82.2	154.6	267.5	313.1	74.7	155.2	181.6	34.1	54.5	71.8	47.0	86.4	97.9	nan	nan	
		6	17.8	24.4		86.9	182.1	343.8	386.2	93.1	187.3	235.6	42.9	71.7	71.8	54.2	101.0	133.3	nan	nan		
		7						233.9	426.9	588.4	145.7	272.0	328.4	54.0	102.0	122.2	70.7	152.7	183.6	nan	nan	
		8						288.8	528.8	606.4	168.1	309.8	381.2	77.1	119.1	135.0	94.6	182.5	230.4	nan	nan	
		9						356.7	659.6	818.5	211.5	406.6	521.6	84.1	160.8	188.6	113.0	226.0	290.3	nan	nan	
		10		77.6					417.7	720.6	929.6	259.3	458.4	578.3	95.8	182.4	224.5	117.5	267.1	359.0	nan	nan
		18						1180.2	2006.3	2540.0	766.4	1417.5	1595.5	315.3	547.1	641.0	381.9	819.1	641.0	nan	nan	
Intramolecular hydrogen bonds	#	3						nan	nan	nan	0.7	0.0	0.6	nan	nan	nan	0.0	0.9	0.1	nan	nan	
		4						nan	nan	nan	0.7	3.9	1.4	nan	nan	nan	0.9	1.8	0.1	nan	nan	
		5						nan	nan	nan	0.8	2.4	0.8	nan	nan	nan	1.8	1.9	0.3	nan	nan	
		6						nan	nan	nan	0.3	1.1	1.9	nan	nan	nan	0.1	0.2	0.3	nan	nan	
		7						nan	nan	nan	1.2	1.4	0.6	nan	nan	nan	0.1	2.1	0.6	nan	nan	
		8						nan	nan	nan	0.8	3.6	1.7	nan	nan	nan	1.0	1.4	0.5	nan	nan	
		9						nan	nan	nan	0.8	3.3	2.4	nan	nan	nan	1.0	4.9	0.5	nan	nan	
		10						nan	nan	nan	1.9	0.8	3.0	nan	nan	nan	0.1	3.5	0.7	nan	nan	
		18						nan	nan	nan	3.7	12.2	11.1	nan	nan	nan	2.3	5.4	0.7	nan	nan	
Charge		3						12	23	34									210			
		4						16	36	49									396			
		5		4	6		14	31	61	80									642			
		6	3	4		15		37	81	101									1140			
		7						46	112	144									1614			
		8						56	134	171									2472			
		9						72	179	226									3246			
		10		13					89	188	259									4560		
		18						275	593	789									23832			