SUPPORTING INFORMATION for Adsorption of PAHs on interstellar ice as viewed by classical molecular dynamics

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- Table S1 lists the quadrupole moment QZZ computed at MP2/cc-pvtz in gas phase and with a PCM (with a dielectric constant of liquid water) for the considered PAHs.

- Tables S2 to S15 associated with figures S1 to S14 list the atoms' coordinates and charges associated with the GOCPAH and SPAHQ model derived for the different PAHs.

- Figure S15 to S22 shows the angular distributions characterizing the orientation of each PAH on the various ice surfaces.

- Figure S23 and S24 correspond respectively to the potential energy surfaces (PESs) obtained for coronene on top of the basal plane of hexagonal ice and amorphous ice after having adjusted the color scale to the maximum of each PES.

Table S1: Quadrupole component along the normal to the molecular plane (Q_{zz}) in Debye/Å calculated in gas phase or with a PCM at MP2/cc-PVTZ level.

	Benzene	Naphthalene	Anthracene	Phenanthrene	Pyrene	Tetracenene	Coronene	Ovalene
gas phase	-7.84	-12.32	-16.91	-16.98	-18.68	-21.60	-27.32	-35.49
PCM	-8.73	-14.17	-19.84	-20.02	-22.30	-25.69	-33.72	-44.70

PAHs XYZ files for the different models, GOCPAH and SPAHQ.

XYZ coordinates are given in angstroms and charges in a.u.

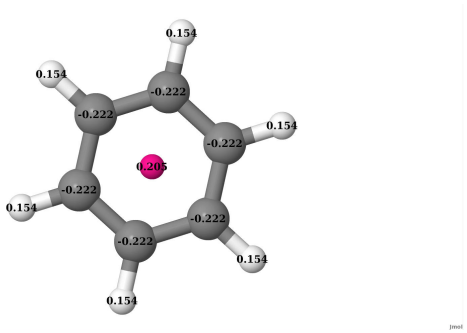

Figure S1: Benzene GOCPAH

14				
Atome Label	X	Y	Z	Partial Charge
C	18.63000	20.08000	20.17000	-0.222
C	19.46000	19.98000	21.28000	-0.222
C	20.83000	19.90000	21.11000	-0.222
C	21.38000	19.93000	19.84000	-0.222
C	20.55000	20.03000	18.73000	-0.222
C	19.18000	20.10000	18.89000	-0.222
H	21.48000	19.82000	21.98000	0.154
H	22.46000	19.87000	19.71000	0.154
H	20.98000	20.05000	17.73000	0.154
H	18.53000	20.18000	18.03000	0.154
H	17.55000	20.14000	20.30000	0.154
H	19.03000	19.96000	22.27000	0.154
Xx	20.01000	20.10000	20.01000	0.204
Xx	20.00000	19.91000	20.00000	0.204

Table S2

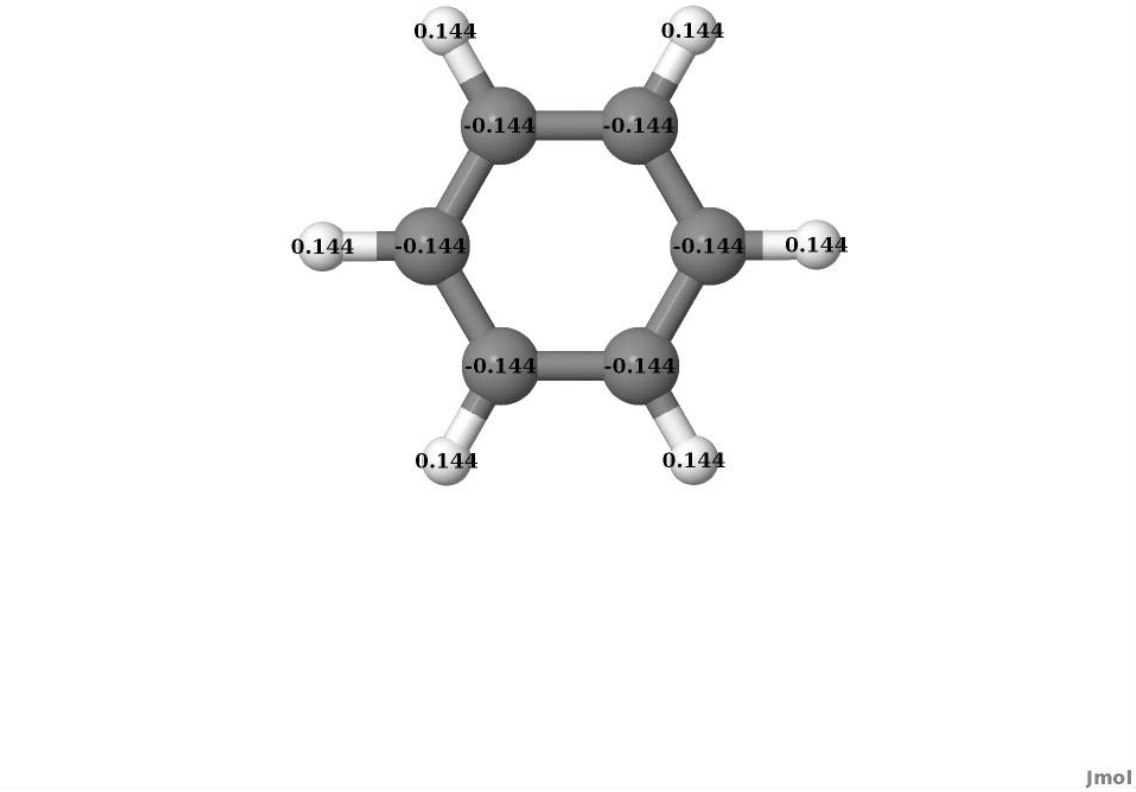

Figure S2: Benzene SPAHQ

12

Atome Label	X	Y	Z	Partial Charge
C	18.80000	20.00000	19.30000	-0.144
C	18.80000	20.00000	20.69000	-0.144
C	20.00000	20.00000	21.38000	-0.144
C	21.20000	20.00000	20.69000	-0.144
C	21.20000	20.00000	19.30000	-0.144
C	20.00000	20.00000	18.61000	-0.144

H	22.14000	20.00000	21.23000	0.144
H	22.14000	20.00000	18.76000	0.144
H	20.00000	20.00000	17.52000	0.144
H	17.85000	20.00000	18.76000	0.144
H	17.85000	20.00000	21.23000	0.144
H	20.00000	20.00000	22.47000	0.144

Table S3

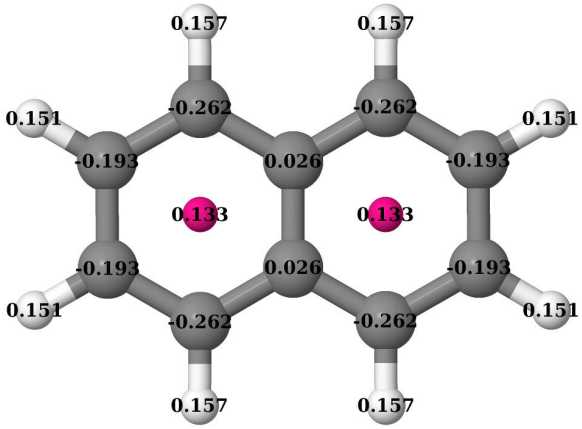

Figure S3: Naphthalene GOCPAH

22

Atome Label	X	Y	Z	Partial Charge
C	18.18000	20.00000	18.27000	-0.193
C	18.20000	20.00000	19.66000	-0.262
C	19.40000	20.00000	20.35000	0.026
C	20.60000	20.00000	19.65000	0.026
C	20.59000	20.00000	18.26000	-0.262
C	19.38000	20.00000	17.57000	-0.193
C	21.80000	20.00000	20.34000	-0.262
C	21.81000	20.00000	21.73000	-0.193
C	20.61000	20.00000	22.43000	-0.193
C	19.41000	20.00000	21.74000	-0.262
H	17.25000	20.00000	20.20000	0.157
H	18.47000	20.00000	22.29000	0.157
H	20.62000	20.00000	23.51000	0.151
H	22.76000	20.00000	22.26000	0.151

H	22.74000	20.00000	19.80000	0.157
H	21.52000	20.00000	17.71000	0.157
H	19.38000	20.00000	16.49000	0.151
H	17.24000	20.00000	17.74000	0.151
Xx	20.60000	19.92000	21.04000	0.134
Xx	20.60000	20.08000	21.04000	0.134
Xx	19.39000	20.08000	18.96000	0.134
Xx	19.39000	19.92000	18.96000	0.134

Table S4

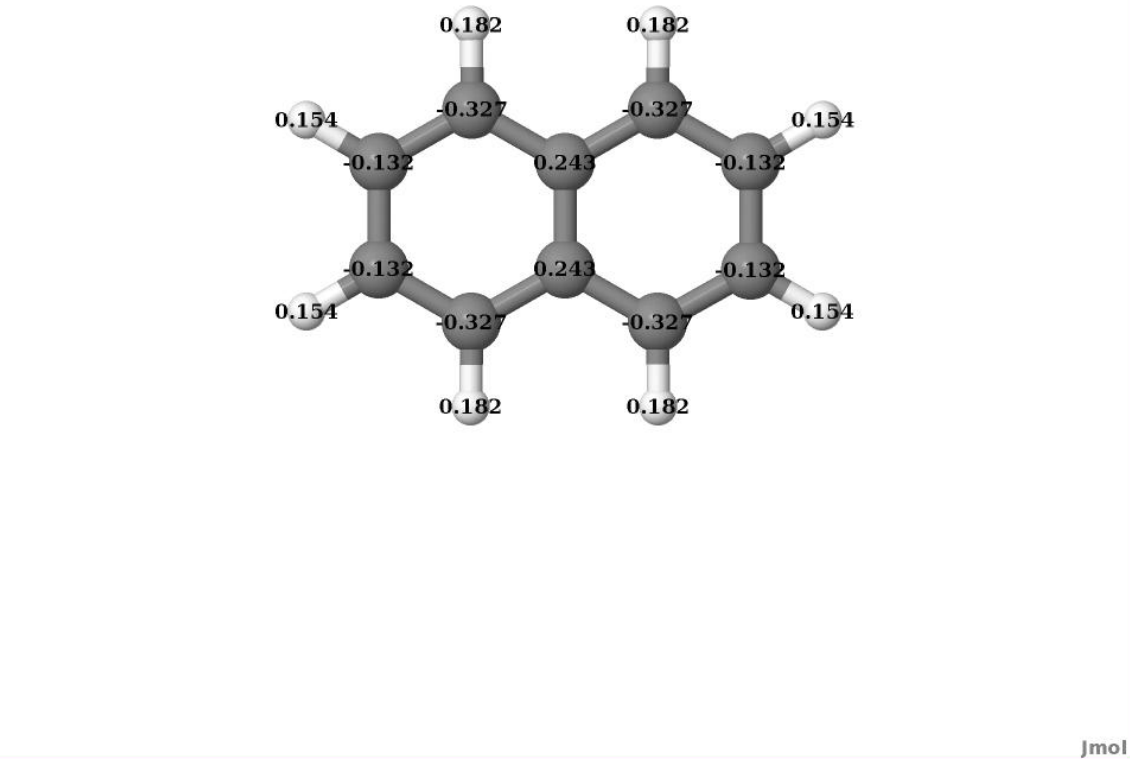

Figure S4: Naphthalene SPAHQ

18

Atome Label	X	Y	Z	Partial Charge
C	18.19000	20.00000	18.27000	-0.132
C	18.20000	20.00000	19.66000	-0.327
C	19.41000	20.00000	20.35000	0.246
C	20.60000	20.00000	19.65000	0.246
C	20.59000	20.00000	18.26000	-0.327
C	19.39000	20.00000	17.57000	-0.132

C	21.81000	20.00000	20.34000	-0.327
C	21.82000	20.00000	21.73000	-0.132
C	20.62000	20.00000	22.43000	-0.132
C	19.42000	20.00000	21.74000	-0.327
H	17.26000	20.00000	20.20000	0.182
H	18.49000	20.00000	22.29000	0.182
H	20.62000	20.00000	23.51000	0.154
H	22.76000	20.00000	22.26000	0.154
H	22.75000	20.00000	19.80000	0.182
H	21.52000	20.00000	17.70000	0.182
H	19.39000	20.00000	16.48000	0.154
H	17.24000	20.00000	17.74000	0.154

Table S5

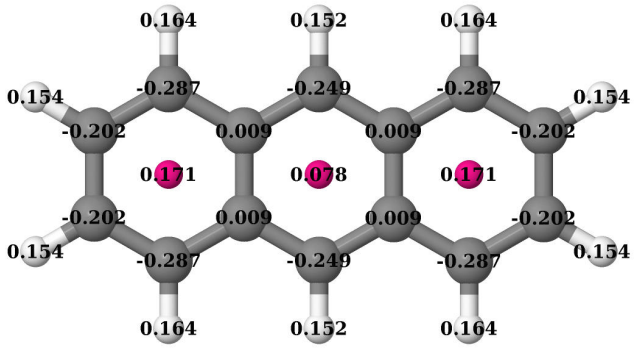

Figure S5: Anthracene GOCPAH

30

Atome Label	X	Y	Z	Partial Charge
C	17.59000	18.62000	20.00000	-0.287745
C	18.80000	19.31000	20.00000	0.009278
C	18.80000	20.69000	20.00000	0.009278
C	17.59000	21.38000	20.00000	-0.287745
C	16.39000	20.69000	20.00000	-0.202796
C	16.39000	19.31000	20.00000	-0.202796
C	20.00000	21.38000	20.00000	-0.249954
C	21.20000	20.69000	20.00000	0.009278
C	21.20000	19.30000	20.00000	0.009278
C	20.00000	18.62000	20.00000	-0.249954
C	22.41000	18.61000	20.00000	-0.287745
C	23.61000	19.30000	20.00000	-0.202796
C	23.61000	20.69000	20.00000	-0.202796
C	22.41000	21.38000	20.00000	-0.287745

H	20.00000	22.47000	20.00000	0.152379
H	22.41000	22.47000	20.00000	0.164504
H	24.55000	21.24000	20.00000	0.154660
H	24.55000	18.76000	20.00000	0.154660
H	22.41000	17.53000	20.00000	0.164504
H	20.00000	17.53000	20.00000	0.152379
H	17.59000	22.47000	20.00000	0.164504
H	15.45000	21.24000	20.00000	0.154660
H	15.45000	18.76000	20.00000	0.154660
H	17.59000	17.53000	20.00000	0.164504
Xx	20.00000	20.00000	20.00000	0.078139
Xx	20.00000	20.00000	20.00000	0.078139
Xx	22.41000	20.00000	19.94000	0.171817
Xx	22.41000	20.00000	20.06000	0.171817
Xx	17.59000	20.00000	19.94000	0.171817
Xx	17.59000	20.00000	20.06000	0.171817

Table S6

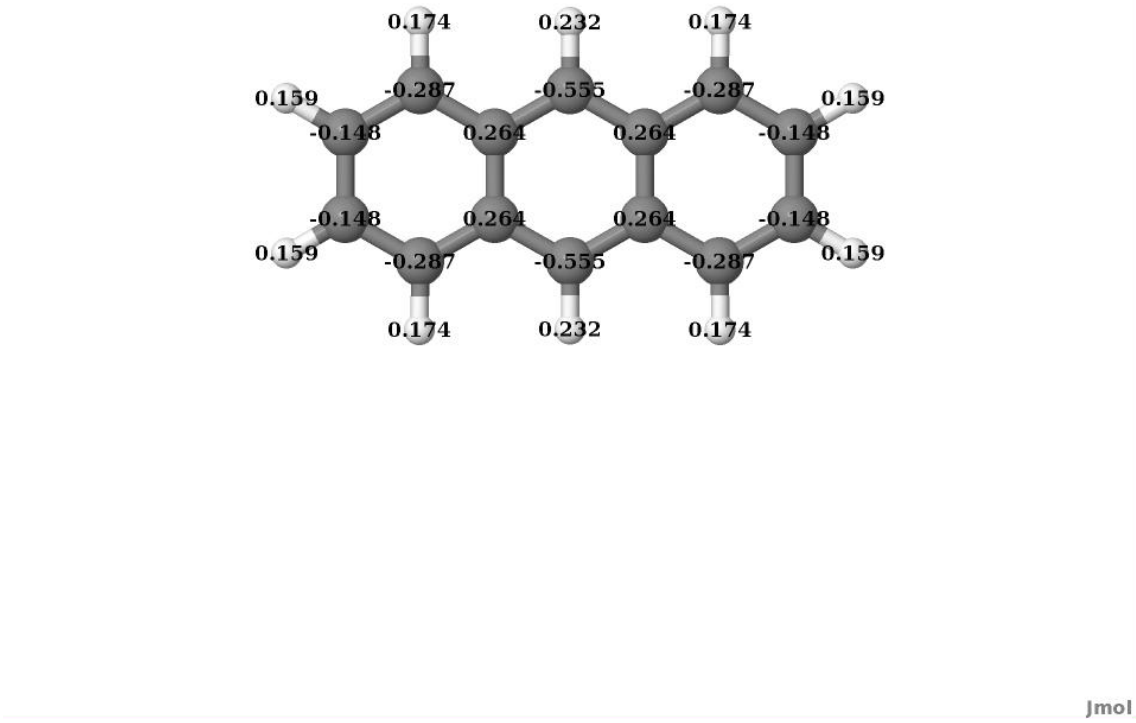

Figure S6: Anthracene SPAHQ

24

Atome Label	X	Y	Z	Partial Charge
C	17.59000	18.62000	20.00000	-0.2877097
C	18.79000	19.31000	20.00000	0.2645268
C	18.79000	20.69000	20.00000	0.2645268
C	17.59000	21.38000	20.00000	-0.2877098
C	16.39000	20.69000	20.00000	-0.1486367
C	16.39000	19.31000	20.00000	-0.1486367

C	20.00000	21.38000	20.00000	-0.5550953
C	21.21000	20.69000	20.00000	0.2645268
C	21.21000	19.31000	20.00000	0.2645268
C	20.00000	18.62000	20.00000	-0.5550953
C	22.41000	18.62000	20.00000	-0.2877098
C	23.61000	19.31000	20.00000	-0.1486367
C	23.61000	20.69000	20.00000	-0.1486367
C	22.41000	21.38000	20.00000	-0.2877098
H	20.00000	22.46000	20.00000	0.2324568
H	22.42000	22.47000	20.00000	0.1740028
H	24.55000	21.24000	20.00000	0.1591361
H	24.55000	18.76000	20.00000	0.1591361
H	22.42000	17.53000	20.00000	0.1740028
H	20.00000	17.54000	20.00000	0.2324568
H	17.58000	22.47000	20.00000	0.1740028
H	15.45000	21.24000	20.00000	0.1591361
H	15.45000	18.76000	20.00000	0.1591361
H	17.58000	17.53000	20.00000	0.1740028

Table S7

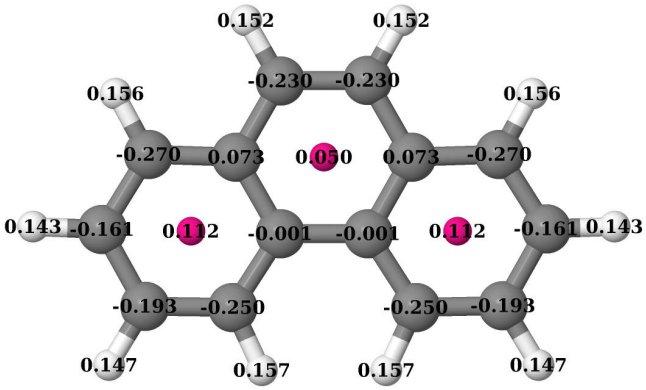

Figure S7: Phenanthrene GOCPAH

30

Atome Label	X	Y	Z	Partial Charge
C	19.31000	19.64000	20.00000	-0.001438
C	18.62000	20.85000	20.00000	0.073981
C	20.70000	19.64000	20.00000	-0.001438
C	19.31000	22.05000	20.00000	-0.230864
C	20.69000	22.06000	20.00000	-0.230864
C	21.38000	20.85000	20.00000	0.073981
C	22.77000	20.89000	20.00000	-0.270068
C	23.51000	19.72000	20.00000	-0.161791
C	22.83000	18.51000	20.00000	-0.193917
C	21.45000	18.48000	20.00000	-0.250043
C	17.23000	20.89000	20.00000	-0.270068
C	16.50000	19.71000	20.00000	-0.161791
C	17.17000	18.50000	20.00000	-0.193917
C	18.56000	18.48000	20.00000	-0.250043

H	19.02000	17.49000	20.00000	0.157342
H	16.61000	17.57000	20.00000	0.147985
H	15.41000	19.75000	20.00000	0.143353
H	16.71000	21.85000	20.00000	0.156428
H	18.77000	23.00000	20.00000	0.152582
H	21.23000	23.00000	20.00000	0.152582
H	23.29000	21.85000	20.00000	0.156428
H	24.59000	19.75000	20.00000	0.143353
H	23.39000	17.57000	20.00000	0.147985
H	20.99000	17.49000	20.00000	0.157342
Xx	20.00000	20.85000	20.03000	0.050559
Xx	20.00000	20.85000	19.97000	0.050559
Xx	17.90000	19.68000	19.96000	0.112945
Xx	17.90000	19.68000	20.04000	0.112945
Xx	22.11000	19.68000	19.96000	0.112945
Xx	22.11000	19.68000	20.04000	0.112945

Table S8

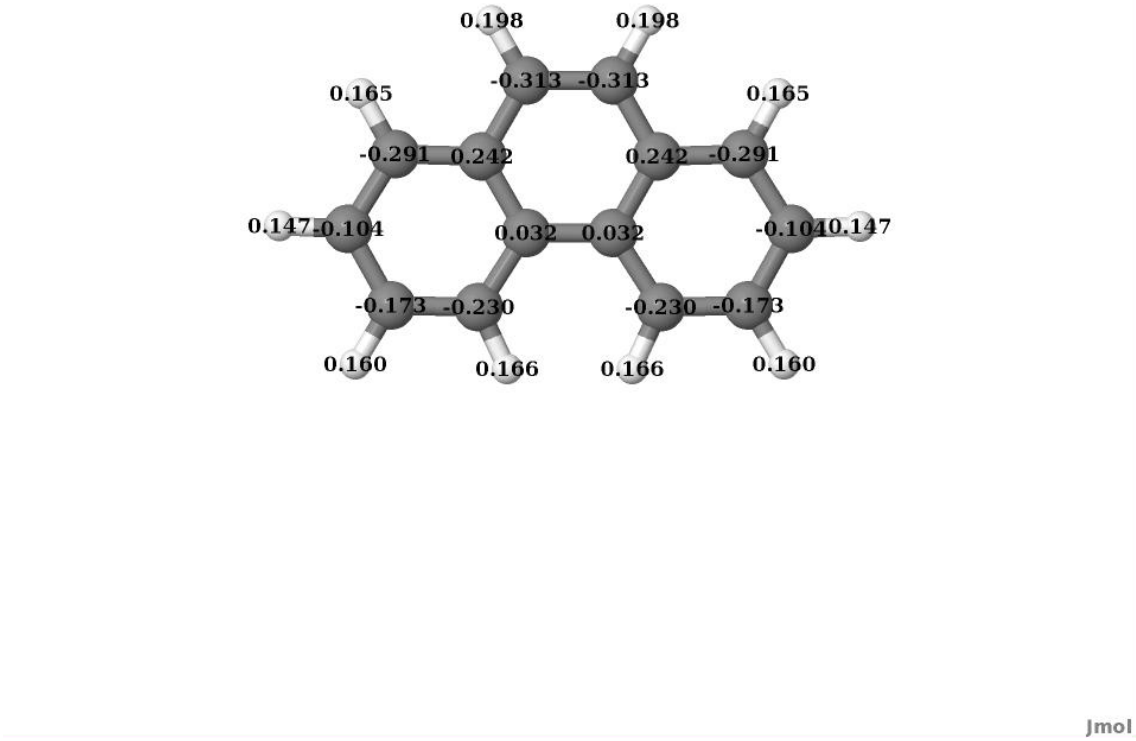

Figure S8: Phenanthrene SPAHQ

24

Atome Label	X	Y	Z	Partial Charge
C	17.59000	18.62000	20.00000	0.0322274
C	18.79000	19.31000	20.00000	0.2425299
C	18.79000	20.69000	20.00000	0.0322274
C	17.59000	21.38000	20.00000	-0.3134567
C	16.39000	20.69000	20.00000	-0.3134567
C	16.39000	19.31000	20.00000	0.2425299

C	20.00000	21.38000	20.00000	-0.2912441
C	21.21000	20.69000	20.00000	-0.1044497
C	21.21000	19.31000	20.00000	-0.1739677
C	20.00000	18.62000	20.00000	-0.2307398
C	22.41000	18.62000	20.00000	-0.2912441
C	23.61000	19.31000	20.00000	-0.1044497
C	23.61000	20.69000	20.00000	-0.1739677
C	22.41000	21.38000	20.00000	-0.2307398
H	20.00000	22.46000	20.00000	0.1661060
H	22.42000	22.47000	20.00000	0.1609740
H	24.55000	21.24000	20.00000	0.1478283
H	24.55000	18.76000	20.00000	0.1656270
H	22.42000	17.53000	20.00000	0.1985653
H	20.00000	17.54000	20.00000	0.1985653
H	17.58000	22.47000	20.00000	0.1656270
H	15.45000	21.24000	20.00000	0.1478283
H	15.45000	18.76000	20.00000	0.1609740
H	17.58000	17.53000	20.00000	0.1661060

Table S9

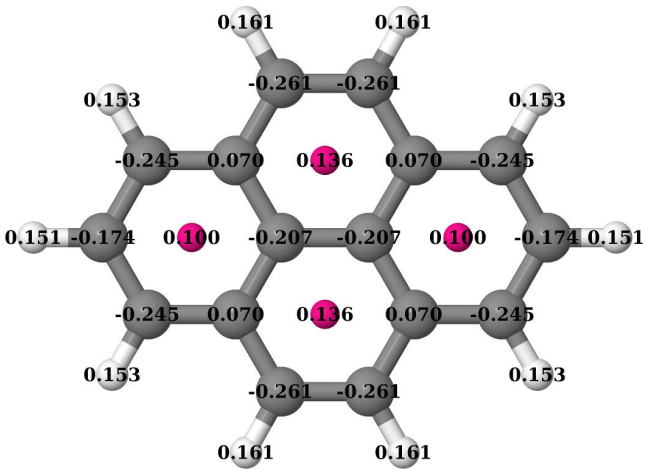

Figure S9: Pyrene GOCPAHQ

34

Atome Label	X	Y	Z	Partial Charge
C	17.23000	18.80000	20.00000	-0.245560
C	18.61000	18.80000	20.00000	0.070441
C	19.31000	20.00000	20.00000	-0.207537
C	18.61000	21.20000	20.00000	0.070441
C	17.23000	21.20000	20.00000	-0.245560
C	16.54000	20.00000	20.00000	-0.174926
C	20.69000	20.00000	20.00000	-0.207537
C	21.39000	21.20000	20.00000	0.070441
C	20.69000	22.40000	20.00000	-0.261263
C	19.31000	22.40000	20.00000	-0.261263
C	21.39000	18.80000	20.00000	0.070441
C	22.77000	18.80000	20.00000	-0.245560
C	23.46000	20.00000	20.00000	-0.174926
C	22.77000	21.20000	20.00000	-0.245560

C	19.31000	17.60000	20.00000	-0.261263
C	20.69000	17.60000	20.00000	-0.261263
H	23.32000	17.86000	20.00000	0.153526
H	24.55000	20.00000	20.00000	0.151523
H	23.32000	22.14000	20.00000	0.153526
H	21.23000	23.35000	20.00000	0.161691
H	18.77000	23.35000	20.00000	0.161691
H	21.23000	16.65000	20.00000	0.161691
H	18.77000	16.65000	20.00000	0.161691
H	16.68000	22.14000	20.00000	0.153526
H	15.45000	20.00000	20.00000	0.151523
H	16.68000	17.86000	20.00000	0.153526
Xx	20.00000	21.20000	20.33000	0.136234
Xx	20.00000	21.20000	19.67000	0.136234
Xx	20.00000	18.80000	20.33000	0.136234
Xx	20.00000	18.80000	19.67000	0.136234
Xx	22.08000	20.00000	20.43000	0.100402
Xx	22.08000	20.00000	19.57000	0.100402
Xx	17.92000	20.00000	19.57000	0.100402
Xx	17.92000	20.00000	20.43000	0.100402

Table S10

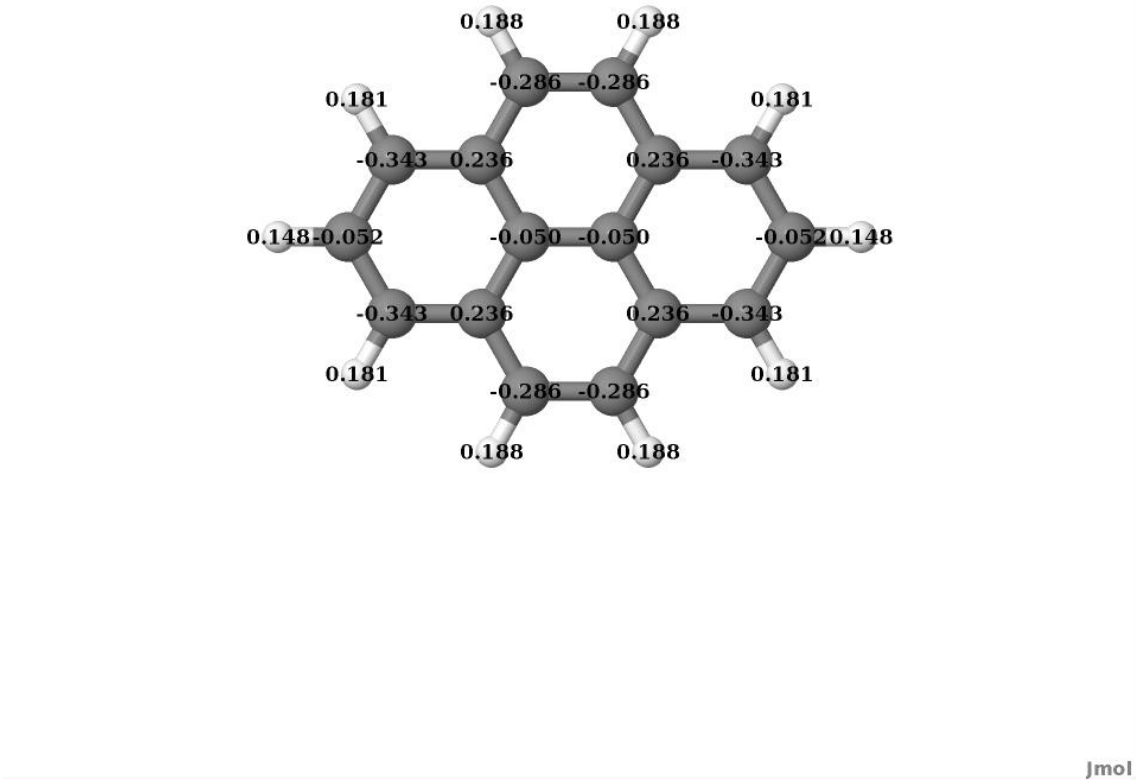

Figure S10: Pyrene SPAHQ

26

Atome Label	X	Y	Z	Partial Charge
C	17.23000	18.80000	20.00000	-0.3434834
C	18.62000	18.80000	20.00000	0.2365414
C	19.31000	20.00000	20.00000	-0.0501761
C	18.62000	21.20000	20.00000	0.2365414
C	17.23000	21.20000	20.00000	-0.3434834
C	16.54000	20.00000	20.00000	-0.0525057

C	20.69000	20.00000	20.00000	-0.0501761
C	21.38000	21.20000	20.00000	0.2365414
C	20.69000	22.41000	20.00000	-0.2865293
C	19.31000	22.41000	20.00000	-0.2865293
C	21.38000	18.80000	20.00000	0.2365414
C	22.77000	18.80000	20.00000	-0.3434834
C	23.46000	20.00000	20.00000	-0.0525057
C	22.77000	21.20000	20.00000	-0.3434834
C	19.31000	17.59000	20.00000	-0.2865293
C	20.69000	17.59000	20.00000	-0.2865293
H	23.32000	17.86000	20.00000	0.1819412
H	24.55000	20.00000	20.00000	0.1483484
H	23.32000	22.14000	20.00000	0.1819412
H	21.23000	23.36000	20.00000	0.1886968
H	18.78000	23.36000	20.00000	0.1886968
H	21.23000	16.64000	20.00000	0.1886968
H	18.78000	16.64000	20.00000	0.1886968
H	16.68000	22.14000	20.00000	0.1819412
H	15.45000	20.00000	20.00000	0.1483484
H	16.68000	17.86000	20.00000	0.1819412

Table S11

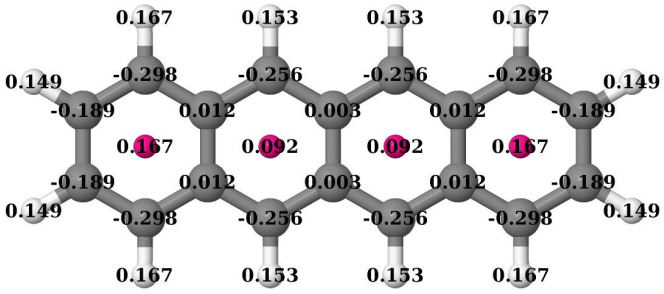

Figure S11: Tetracene GOCPAHQ

38

Atome Label	X	Y	Z	Partial Charge
C	20.00000	20.69000	20.00000	0.003804
C	20.00000	19.31000	20.00000	0.003804
C	18.80000	18.62000	20.00000	-0.256990
C	21.20000	18.62000	20.00000	-0.256990
C	21.20000	21.38000	20.00000	-0.256990
C	18.80000	21.38000	20.00000	-0.256990
C	17.59000	19.31000	20.00000	0.012193
C	22.41000	19.31000	20.00000	0.012193
C	22.41000	20.69000	20.00000	0.012193
C	17.59000	20.69000	20.00000	0.012193
C	16.39000	18.62000	20.00000	-0.298122
C	23.61000	18.62000	20.00000	-0.298122
C	23.61000	21.38000	20.00000	-0.298122
C	16.39000	21.38000	20.00000	-0.298122

C	15.19000	19.31000	20.00000	-0.189195
C	24.82000	19.31000	20.00000	-0.189195
C	24.82000	20.69000	20.00000	-0.189195
C	15.19000	20.69000	20.00000	-0.189195
H	18.80000	17.53000	20.00000	0.153289
H	21.20000	17.53000	20.00000	0.153289
H	21.20000	22.47000	20.00000	0.153289
H	18.80000	22.47000	20.00000	0.153289
H	16.38000	17.53000	20.00000	0.167217
H	23.62000	17.53000	20.00000	0.167217
H	23.62000	22.47000	20.00000	0.167217
H	16.38000	22.47000	20.00000	0.167217
H	14.25000	18.76000	20.00000	0.149028
H	25.75000	18.76000	20.00000	0.149028
H	25.75000	21.24000	20.00000	0.149028
H	14.25000	21.24000	20.00000	0.149028
Xx	18.80000	20.00000	19.94000	0.092722
Xx	18.80000	20.00000	20.07000	0.092722
Xx	21.20000	20.00000	19.94000	0.092722
Xx	21.20000	20.00000	20.06000	0.092722
Xx	23.61000	20.00000	19.91000	0.167956
Xx	23.61000	20.00000	20.09000	0.167956
Xx	16.39000	20.00000	19.91000	0.167956
Xx	16.39000	20.00000	20.09000	0.167956

Table S12

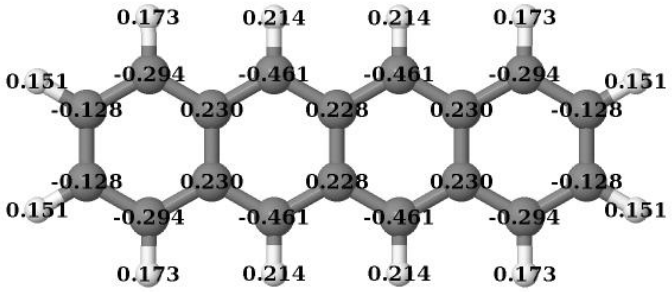

Figure S12: Tetracene SPAHQ

30

Atome Label	X	Y	Z	Partial Charge
C	20.00000	20.69000	20.00000	0.2288471
C	20.00000	19.31000	20.00000	0.2288471
C	18.79000	18.62000	20.00000	-0.4616148
C	21.21000	18.62000	20.00000	-0.4616148
C	21.21000	21.38000	20.00000	-0.4616148
C	18.79000	21.38000	20.00000	-0.4616148

C	17.59000	19.31000	20.00000	0.2309908
C	22.41000	19.31000	20.00000	0.2309908
C	22.41000	20.69000	20.00000	0.2309908
C	17.59000	20.69000	20.00000	0.2309908
C	16.38000	18.62000	20.00000	-0.2943359
C	23.62000	18.62000	20.00000	-0.2943359
C	23.62000	21.38000	20.00000	-0.2943359
C	16.39000	21.38000	20.00000	-0.2943359
C	15.18000	19.31000	20.00000	-0.1289799
C	24.82000	19.31000	20.00000	-0.1289799
C	24.82000	20.69000	20.00000	-0.1289799
C	15.18000	20.69000	20.00000	-0.1289799
H	18.79000	17.54000	20.00000	0.2144502
H	21.21000	17.54000	20.00000	0.2144502
H	21.21000	22.46000	20.00000	0.2144502
H	18.79000	22.46000	20.00000	0.2144502
H	16.37000	17.53000	20.00000	0.1739227
H	23.63000	17.53000	20.00000	0.1739227
H	23.63000	22.47000	20.00000	0.1739227
H	16.37000	22.47000	20.00000	0.1739227
H	14.24000	18.76000	20.00000	0.1511433
H	25.76000	18.76000	20.01000	0.1511433
H	25.76000	21.24000	20.00000	0.1511433
H	14.24000	21.24000	19.99000	0.1511433

Table S13

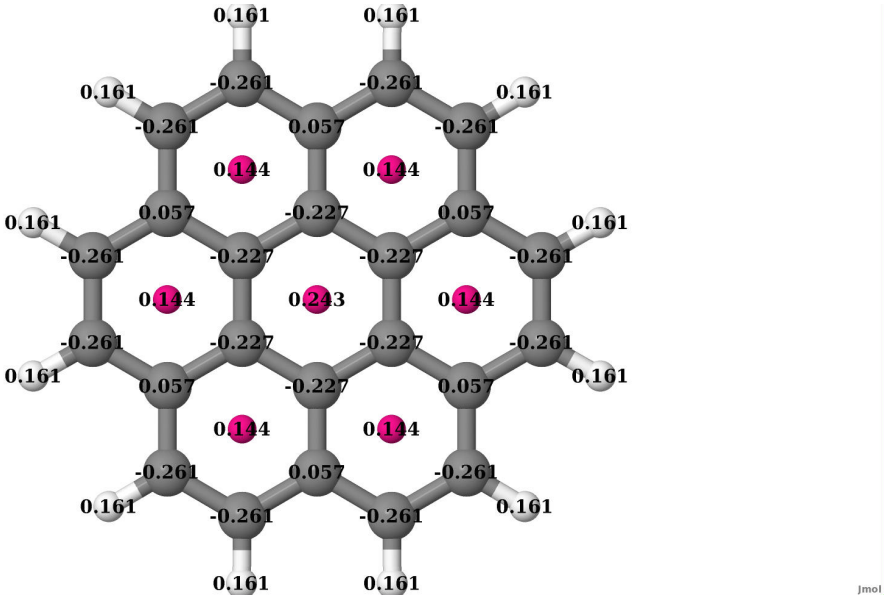

Figure S13: Coronene GOCPAH

50

Atome Label	X	Y	Z	Partial Charge
C	23.42000	19.31000	24.62000	-0.2276849
C	23.42000	20.69000	24.62000	-0.2276834
C	24.62000	21.39000	24.62000	-0.2276834
C	25.82000	20.69000	24.62000	-0.2276834
C	25.82000	19.31000	24.62000	-0.2276834
C	24.62000	18.61000	24.62000	-0.2276834
C	22.22000	18.61000	24.62000	0.0571640
C	22.22000	21.39000	24.62000	0.0571640
C	24.62000	22.77000	24.62000	0.0571640
C	27.02000	21.39000	24.62000	0.0571640
C	27.02000	18.61000	24.62000	0.0571640
C	24.62000	17.23000	24.62000	0.0571640
C	25.82000	23.47000	24.62000	-0.2612067
C	27.03000	22.77000	24.62000	-0.2612067

C	28.23000	20.69000	24.62000	-0.2612067
C	28.23000	19.31000	24.62000	-0.2612067
C	27.02000	17.23000	24.62000	-0.2612067
C	25.82000	16.53000	24.62000	-0.2612067
C	22.22000	17.23000	24.62000	-0.2612067
C	23.42000	16.53000	24.62000	-0.2612067
C	21.02000	19.31000	24.62000	-0.2612067
C	21.02000	20.69000	24.62000	-0.2612067
C	22.22000	22.77000	24.62000	-0.2612067
C	23.42000	23.47000	24.62000	-0.2612067
H	25.83000	24.55000	24.62000	0.1612028
H	27.96000	23.32000	24.62000	0.1612028
H	29.17000	21.23000	24.62000	0.1612028
H	29.17000	18.77000	24.62000	0.1612028
H	27.96000	16.68000	24.62000	0.1612028
H	25.83000	15.45000	24.62000	0.1612028
H	21.28000	16.68000	24.62000	0.1612028
H	23.41000	15.45000	24.62000	0.1612028
H	20.07000	18.77000	24.62000	0.1612028
H	20.07000	21.23000	24.62000	0.1612028
H	21.28000	23.32000	24.62000	0.1612028
H	23.42000	24.55000	24.62000	0.1612028
Xx	24.62000	20.00000	24.68000	0.2435988
Xx	24.62000	20.00000	24.56000	0.2435988
Xx	22.22000	20.00000	24.70000	0.1446703
Xx	22.22000	20.00000	24.54000	0.1446703
Xx	23.42000	17.92000	24.70000	0.1446703

Xx	23.42000	17.92000	24.54000	0.1446703
Xx	25.82000	17.92000	24.70000	0.1446703
Xx	25.82000	17.92000	24.54000	0.1446703
Xx	27.02000	20.00000	24.70000	0.1446703
Xx	27.02000	20.00000	24.54000	0.1446703
Xx	25.82000	22.08000	24.70000	0.1446703
Xx	25.82000	22.08000	24.54000	0.1446703
Xx	23.42000	22.08000	24.54000	0.1446703
Xx	23.42000	22.08000	24.70000	0.1446703

Table S14

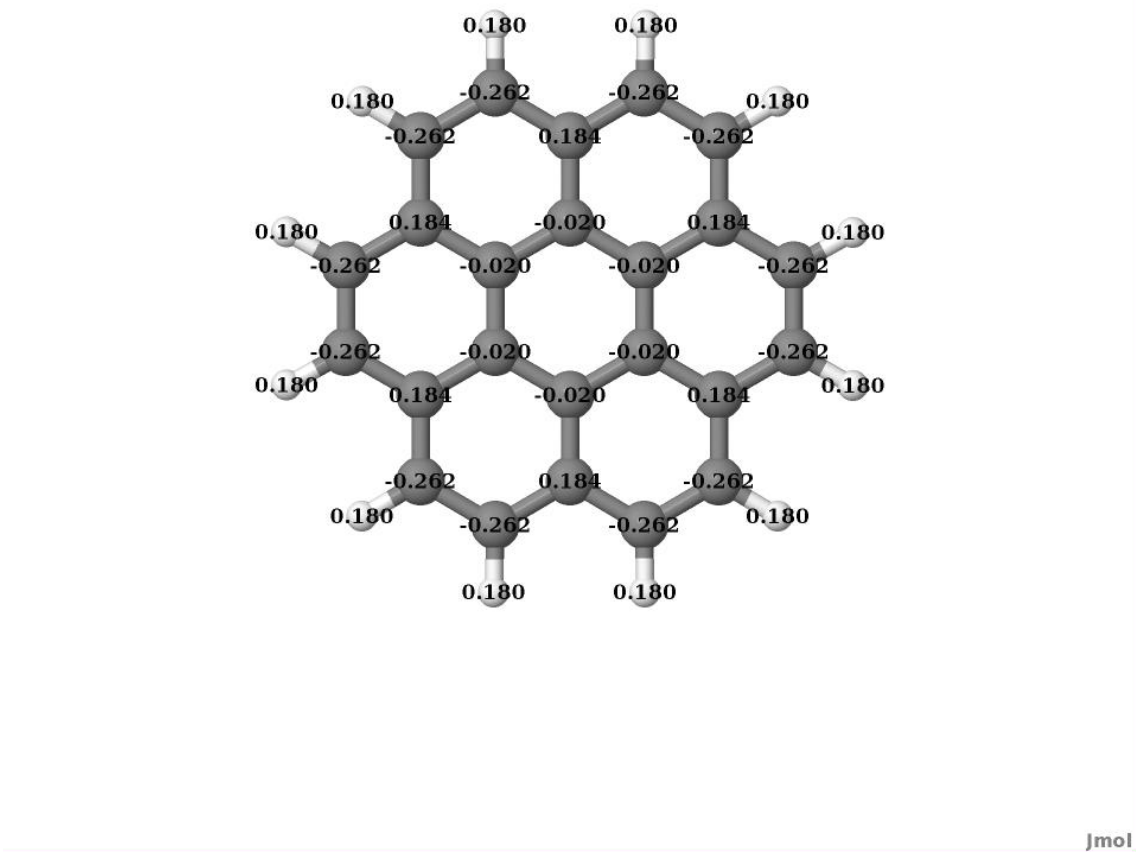

Figure S14: Coronene SPAHQ

36

Atome Label	X	Y	Z	Partial Charge
C	18.80000	19.31000	20.00000	-0.0203804
C	18.80000	20.69000	20.00000	-0.0203805
C	20.00000	21.39000	20.00000	-0.0203805
C	21.20000	20.69000	20.00000	-0.0203805
C	21.20000	19.31000	20.00000	-0.0203805
C	20.00000	18.61000	20.00000	-0.0203805

C	17.60000	18.61000	20.00000	0.1843738
C	17.60000	21.39000	20.00000	0.1843738
C	20.00000	22.77000	20.00000	0.1843738
C	22.40000	21.39000	20.00000	0.1843738
C	22.40000	18.61000	20.00000	0.1843738
C	20.00000	17.23000	20.00000	0.1843738
C	21.20000	23.47000	20.00000	-0.2623178
C	22.40000	22.77000	20.00000	-0.2623178
C	23.60000	20.69000	20.00000	-0.2623178
C	23.60000	19.31000	20.00000	-0.2623178
C	22.40000	17.23000	20.00000	-0.2623178
C	21.20000	16.53000	20.00000	-0.2623178
C	17.60000	17.23000	20.00000	-0.2623178
C	18.80000	16.53000	20.00000	-0.2623178
C	16.40000	19.31000	20.00000	-0.2623178
C	16.40000	20.69000	20.00000	-0.2623178
C	17.60000	22.77000	20.00000	-0.2623178
C	18.80000	23.47000	20.00000	-0.2623178
H	21.22000	24.55000	20.00000	0.1803211
H	23.34000	23.33000	20.00000	0.1803211
H	24.55000	21.22000	20.00000	0.1803211
H	24.55000	18.77000	20.00000	0.1803211
H	23.34000	16.67000	20.00000	0.1803211
H	21.21000	15.45000	20.00000	0.1803211
H	16.66000	16.67000	20.00000	0.1803211
H	18.78000	15.45000	20.00000	0.1803211
H	15.45000	18.78000	20.00000	0.1803211

H	15.45000	21.23000	20.00000	0.1803211
H	16.67000	23.33000	20.00000	0.1803211
H	18.79000	24.55000	20.00000	0.1803211

Table S15

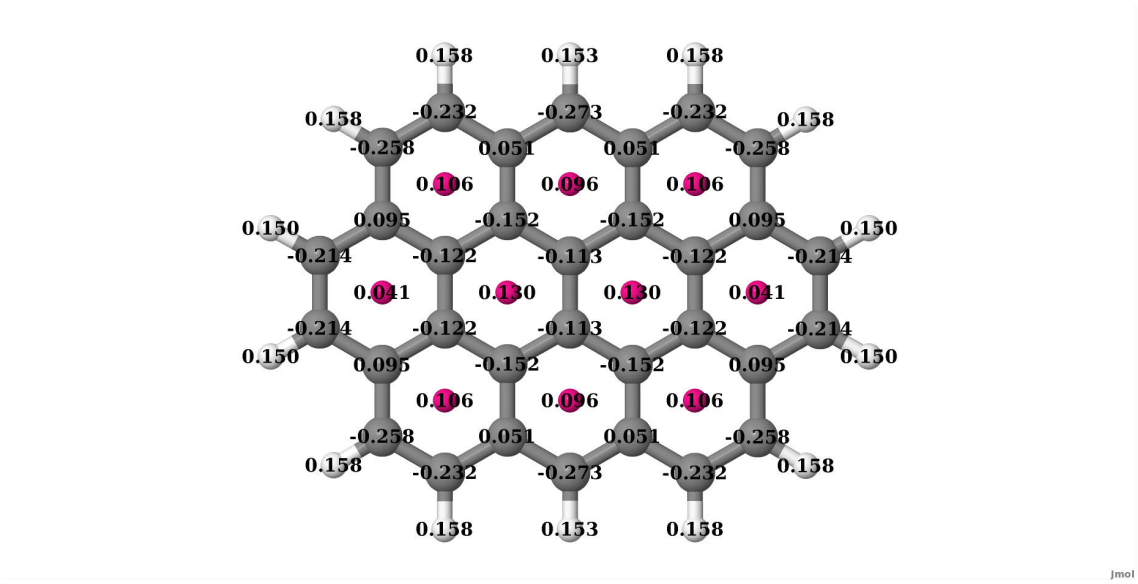

Figure S15: Ovalene GOCPAHQ

66

Atome Label	X	Y	Z	Partial Charge
C	17.60000	23.47000	20.00000	-0.2327535
C	18.80000	22.77000	20.00000	0.0512503
C	18.80000	21.39000	20.00000	-0.1520033
C	17.60000	20.70000	20.00000	-0.1221014
C	16.40000	21.39000	20.00000	0.0959647
C	16.40000	22.78000	20.00000	-0.2583554
C	20.00000	20.69000	20.00000	-0.1139892
C	20.00000	19.31000	20.00000	-0.1139892
C	18.80000	18.62000	20.00000	-0.1520033
C	17.60000	19.31000	20.00000	-0.1221014
C	18.80000	17.23000	20.00000	0.0512503
C	20.00000	16.54000	20.00000	-0.2730198
C	21.20000	17.23000	20.00000	0.0512503
C	21.20000	18.61000	20.00000	-0.1520033

C	22.40000	19.31000	20.00000	-0.1221014
C	23.61000	18.61000	20.00000	0.0959647
C	23.61000	17.22000	20.00000	-0.2583554
C	22.40000	16.53000	20.00000	-0.2327535
C	22.40000	20.69000	20.00000	-0.1221014
C	23.61000	21.39000	20.00000	0.0959647
C	24.81000	20.69000	20.00000	-0.2142686
C	24.81000	19.30000	20.00000	-0.2142686
C	21.20000	21.39000	20.00000	-0.1520033
C	16.39000	18.61000	20.00000	0.0959647
C	16.39000	17.23000	20.00000	-0.2583554
C	17.60000	16.54000	20.00000	-0.2327535
C	21.20000	22.77000	20.00000	0.0512503
C	22.41000	23.47000	20.00000	-0.2327535
C	23.61000	22.77000	20.00000	-0.2583554
C	15.19000	20.70000	20.00000	-0.2142686
C	15.19000	19.31000	20.00000	-0.2142686
C	20.00000	23.46000	20.00000	-0.2730198
H	22.41000	15.45000	20.00000	0.1581759
H	24.54000	16.67000	20.00000	0.1587673
H	25.75000	18.77000	20.00000	0.1507619
H	20.00000	15.45000	20.00000	0.1536782
H	17.59000	15.45000	20.00000	0.1581759
H	15.46000	16.68000	20.00000	0.1587673
H	22.41000	24.55000	20.00000	0.1581759
H	14.25000	21.23000	20.00000	0.1507619
H	15.46000	23.33000	20.00000	0.1587673

H	17.59000	24.55000	20.00000	0.1581759
H	25.75000	21.23000	20.00000	0.1507619
H	20.00000	24.55000	20.00000	0.1536782
H	14.25000	18.77000	20.00000	0.1507619
H	24.54000	23.32000	20.00000	0.1587673
Xx	18.80000	20.00000	19.51000	0.1309765
Xx	18.80000	20.00000	20.49000	0.1309765
Xx	21.20000	20.00000	19.51000	0.1309765
Xx	21.20000	20.00000	20.49000	0.1309765
Xx	16.40000	20.00000	20.97000	0.0416123
Xx	16.40000	20.00000	19.03000	0.0416123
Xx	23.61000	20.00000	19.03000	0.0416123
Xx	23.61000	20.00000	20.97000	0.0416123
Xx	20.00000	17.92000	20.00000	0.0964023
Xx	20.00000	17.92000	20.00000	0.0964023
Xx	20.00000	22.08000	20.00000	0.0964023
Xx	20.00000	22.08000	20.00000	0.0964023
Xx	22.40000	17.92000	20.00000	0.1061182
Xx	22.40000	17.92000	20.00000	0.1061182
Xx	22.41000	22.08000	20.00000	0.1061182
Xx	22.41000	22.08000	20.00000	0.1061182
Xx	17.60000	22.08000	20.00000	0.1061182
Xx	17.60000	22.08000	20.00000	0.1061182
Xx	17.60000	17.92000	20.00000	0.1061182
Xx	17.60000	17.92000	20.00000	0.1061182

Table S16

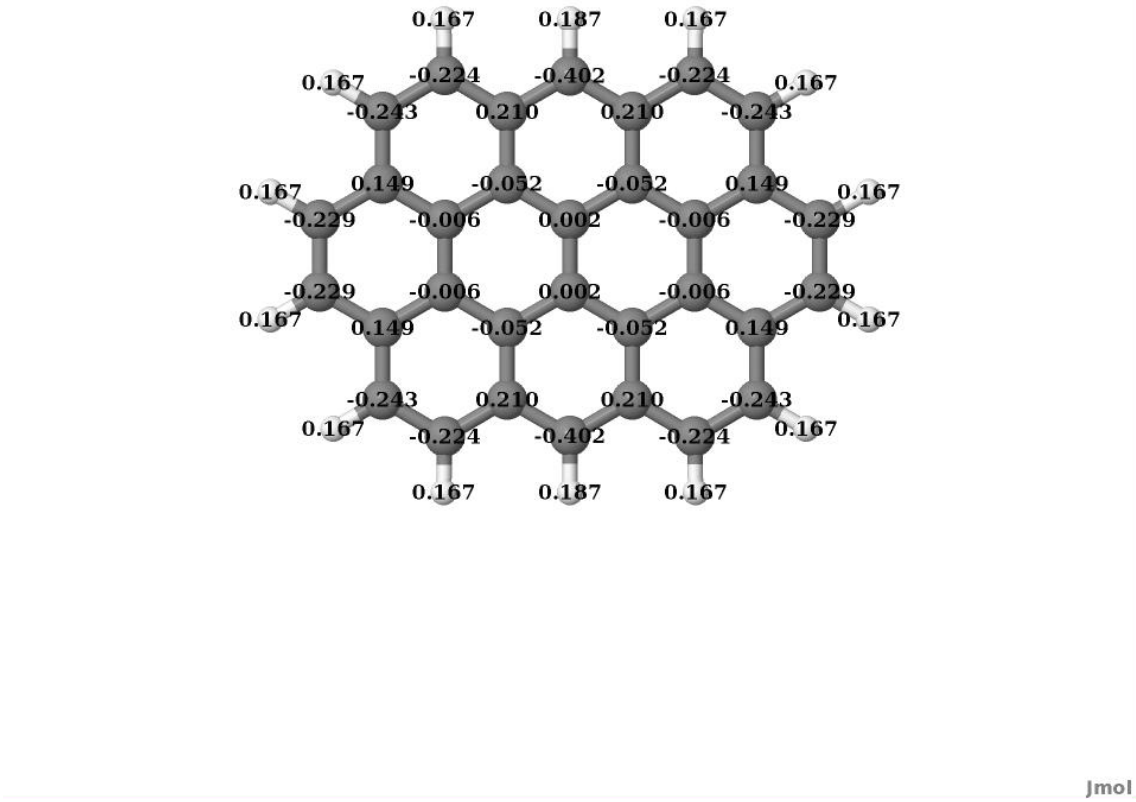

Figure S16: Ovalene SPAHQ

46

Atome Label	X	Y	Z	Partial Charge
C	17.60000	23.47000	20.00000	-0.2244004
C	18.80000	22.77000	20.00000	0.2102151
C	18.80000	21.39000	20.00000	-0.0520617
C	17.60000	20.69000	20.00000	-0.0064924
C	16.40000	21.39000	20.00000	0.1497546
C	16.40000	22.77000	20.00000	-0.2430910

C	20.00000	20.69000	20.00000	0.0020516
C	20.00000	19.31000	20.00000	0.0020516
C	18.80000	18.61000	20.00000	-0.0520617
C	17.60000	19.31000	20.00000	-0.0064924
C	18.80000	17.23000	20.00000	0.2102151
C	20.00000	16.54000	20.00000	-0.4022495
C	21.20000	17.23000	20.00000	0.2102151
C	21.20000	18.61000	20.00000	-0.0520617
C	22.40000	19.31000	20.00000	-0.0064924
C	23.60000	18.61000	20.00000	0.1497546
C	23.60000	17.23000	20.00000	-0.2430910
C	22.40000	16.53000	20.00000	-0.2244004
C	22.40000	20.69000	20.00000	-0.0064924
C	23.60000	21.39000	20.00000	0.1497546
C	24.81000	20.69000	20.00000	-0.2294597
C	24.81000	19.31000	20.00000	-0.2294597
C	21.20000	21.39000	20.00000	-0.0520617
C	16.40000	18.61000	20.00000	0.1497546
C	16.40000	17.23000	20.00000	-0.2430910
C	17.60000	16.53000	20.00000	-0.2244004
C	21.20000	22.77000	20.00000	0.2102151
C	22.40000	23.47000	20.00000	-0.2244004
C	23.60000	22.77000	20.00000	-0.2430910
C	15.19000	20.69000	20.00000	-0.2294597
C	15.19000	19.31000	20.00000	-0.2294597
C	20.00000	23.46000	20.00000	-0.4022495
H	22.42000	15.45000	20.00000	0.1670582

H	24.54000	16.67000	20.00000	0.1675817
H	25.75000	18.77000	20.00000	0.1670933
H	20.00000	15.45000	20.00000	0.1878025
H	17.58000	15.45000	20.00000	0.1670582
H	15.46000	16.67000	20.00000	0.1675817
H	22.42000	24.55000	20.00000	0.1670582
H	14.25000	21.23000	20.00000	0.1670933
H	15.46000	23.33000	20.00000	0.1675817
H	17.58000	24.55000	20.00000	0.1670582
H	25.75000	21.23000	20.00000	0.1670933
H	20.00000	24.55000	20.00000	0.1878025
H	14.25000	18.77000	20.00000	0.1670933
H	24.54000	23.33000	20.00000	0.1675817

Table S17

Angular distributions of PAHs adsorbed on various ices.

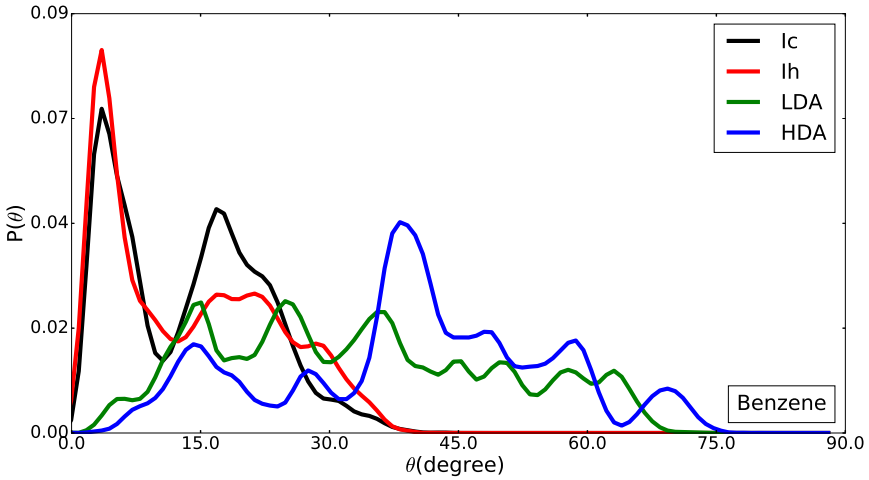

Figure S17: Angular distribution of benzene adsorbedon the various ices. The characterized angle is defined as the angle between the normal to the PAH plane and the surface normal (z axis).

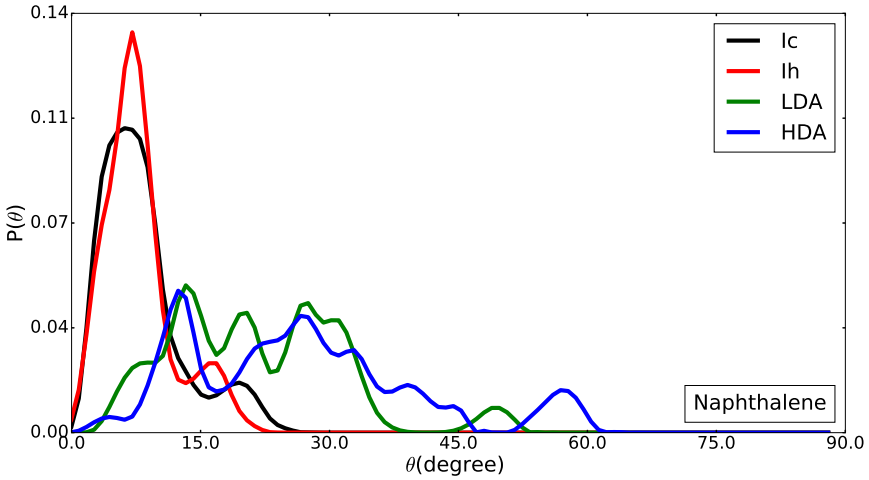

Figure S18: Angular distribution of naphthalene adsorbed on the various ices. The characterized angle is defined as the angle between the normal to the PAH plane and the surface normal (z axis).

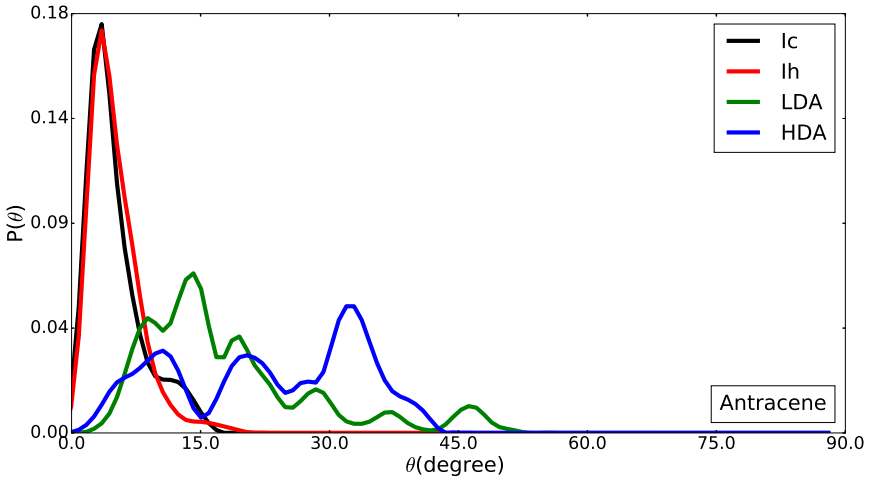

Figure S19: Angular distribution of antracene adsorbed on the various ices. The characterized angle is defined as the angle between the normal to the PAH plane and the surface normal (z axis).

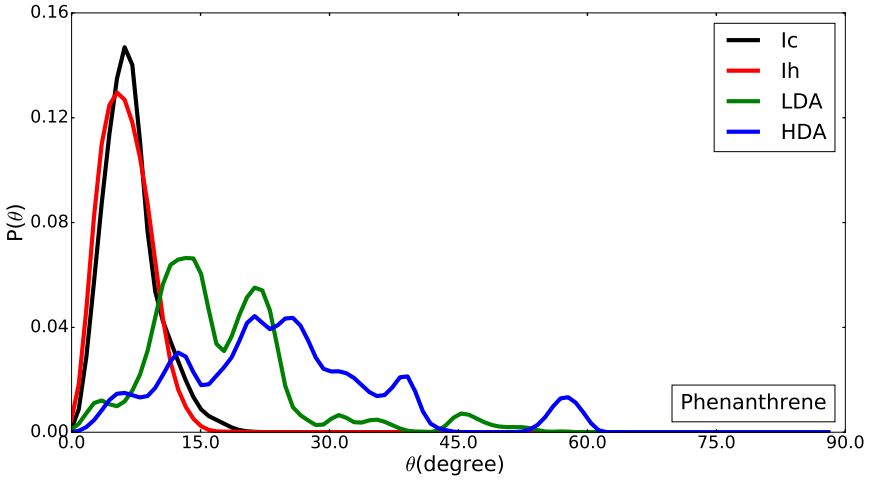

Figure S20: Angular distribution of phenanthrene adsorbed on the various ices. The characterized angle is defined as the angle between the normal to the PAH plane and the surface normal (z axis).

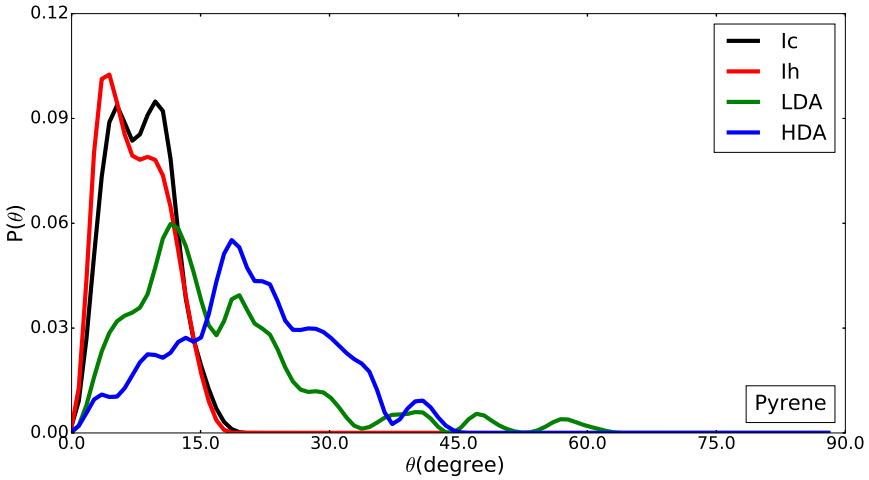

Figure S21: Angular distribution of pyrene adsorbed on the various ices. The characterized angle is defined as the angle between the normal to the PAH plane and the surface normal (z axis).

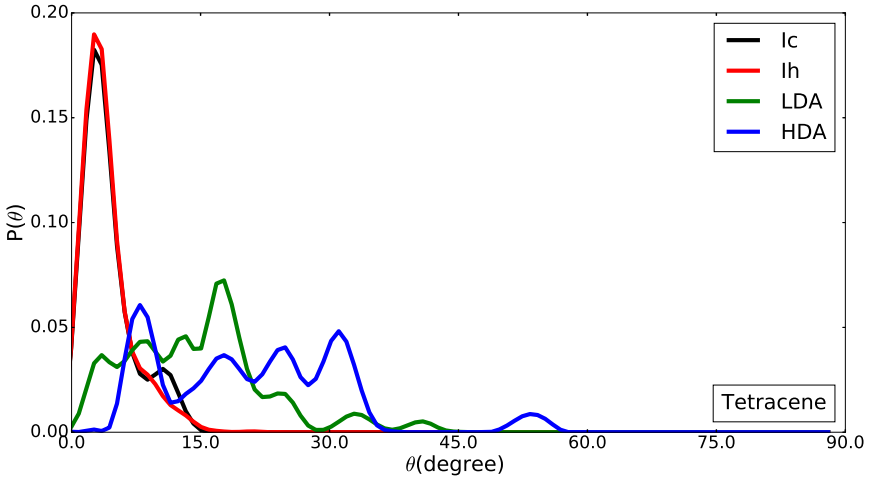

Figure S22: Angular distribution of tetracene adsorbed on the various ices. The characterized angle is defined as the angle between the normal to the PAH plane and the surface normal (z axis).

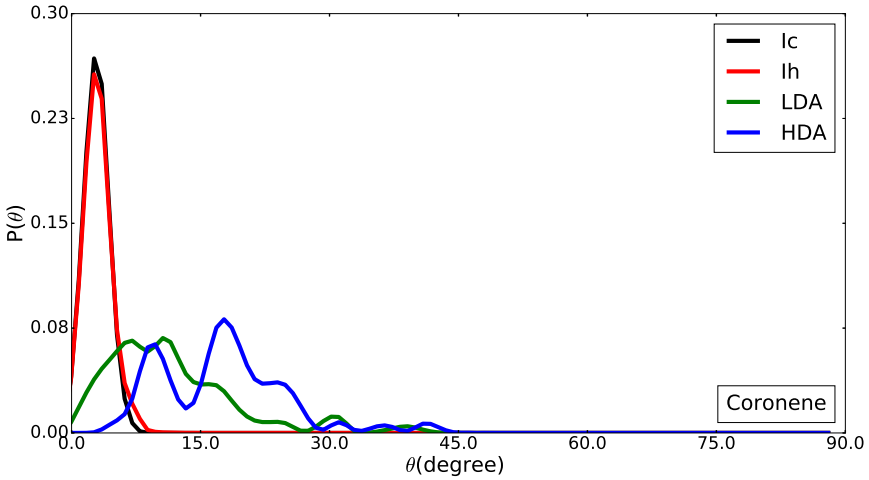

Figure S23: Angular distribution of coronene adsorbed on the various ices. The characterized angle is defined as the angle between the normal to the PAH plane and the surface normal (z axis).

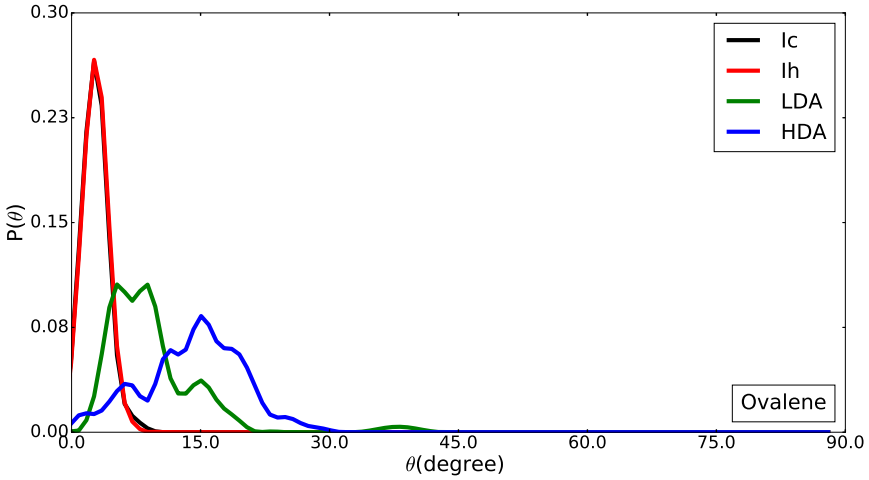

Figure S24: Angular distribution of ovalene adsorbed on the various ices. The characterized angle is defined as the angle between the normal to the PAH plane and the surface normal (z axis).

SEPI between coronene Ih and LDA (amorphous ice).

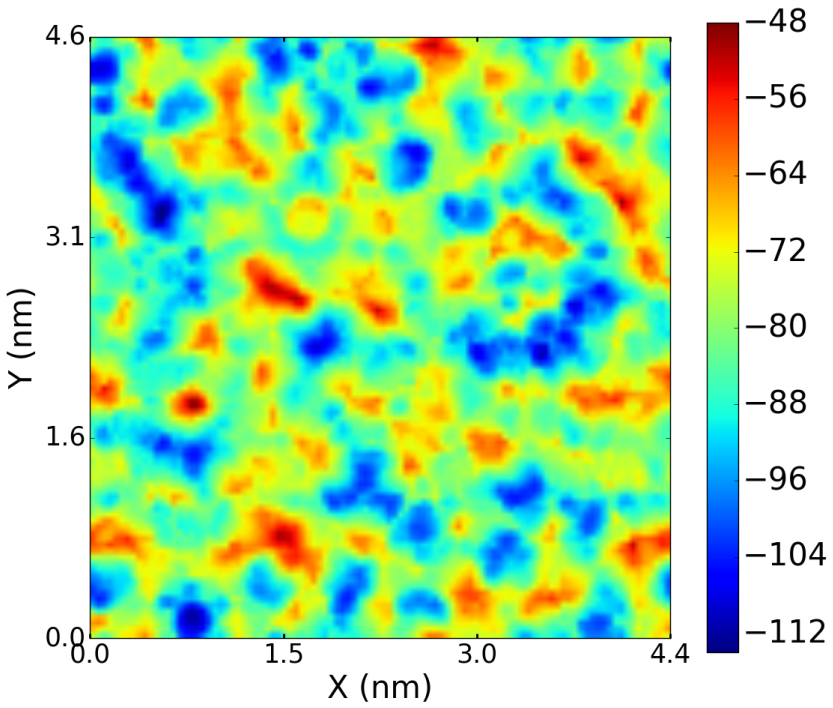

Figure S25: Potential energy surface for coronene on top of the basal plane of hexagonal ice with a better contrast.

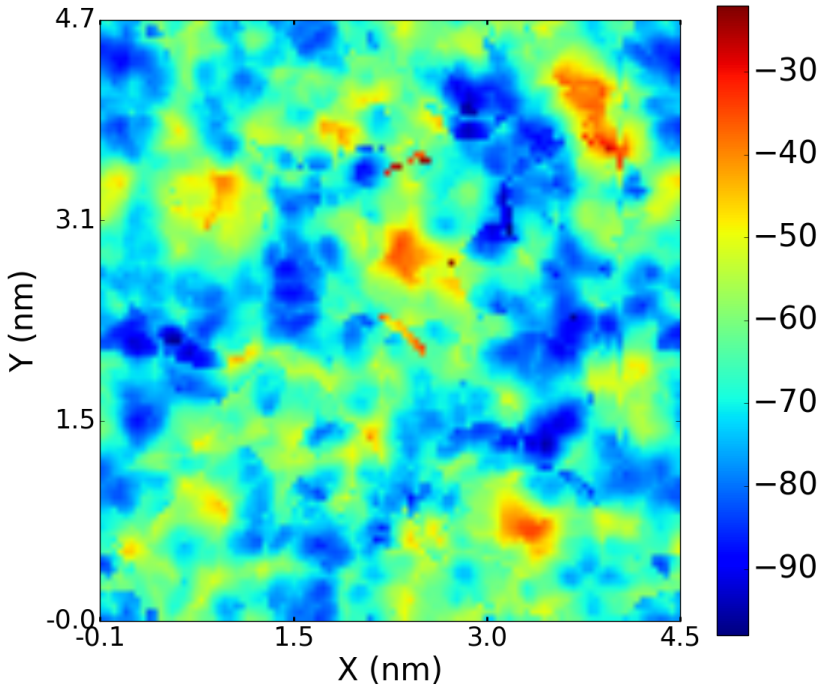

Figure S26: Potential energy surface for coronene on top of amorphous ice with a better contrast.