Supporting Information

Molecular Simulations of The Thermophysical Properties of Polyethylene Glycol Siloxane (PEGS) Solvent for Pre-combustion CO_2 Capture

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1 Classical Force Field Parameters for PEGS

The PEGS molecule is shown in Figure S1.

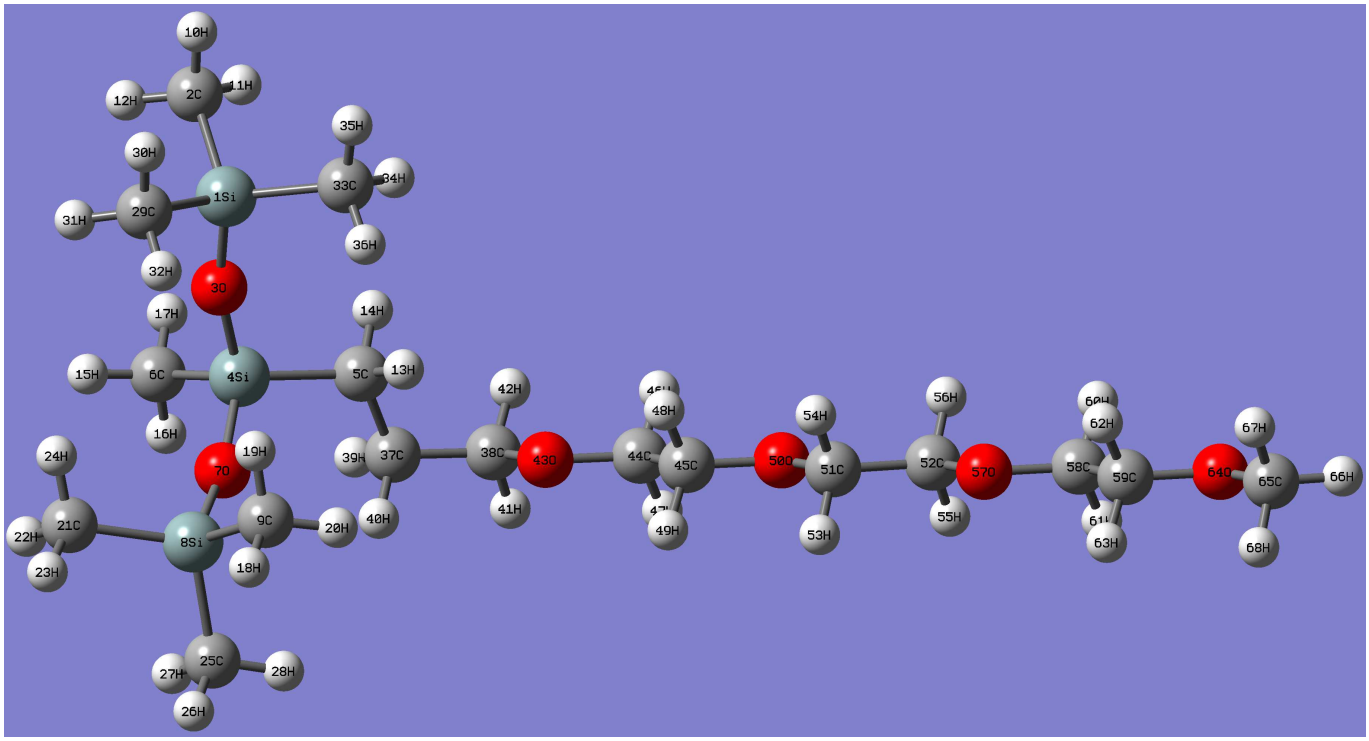

Figure S1: The picture for PEGS molecule with atom number and atom symbol.

The PSF file for a single PEGS molecule is given below. In the "NATOM" part, it contains the atom number (column 1), atom type (column 6), which represents different atom types used in the classical FF parameter part (below); atom charge (column 7), and atom mass (column 8). The PSF file also contains the information for the BOND, ANGLE, DIHEDRAL, and IMPROPER parts.

68 !NATOM

1	HYB	1	HYB	Si	aDSI	1.036000	28.0855	0
2	HYB	1	HYB	C	aDC	-0.506500	12.0107	0
3	HYB	1	HYB	O	aDO	-0.687500	15.9994	0
4	HYB	1	HYB	Si	aDSI	1.019000	28.0855	0
5	HYB	1	HYB	C	aDC	-0.260000	12.0107	0
6	HYB	1	HYB	C	aDC	-0.514000	12.0107	0
7	HYB	1	HYB	O	aDO	-0.687500	15.9994	0
8	HYB	1	HYB	Si	aDSI	1.036000	28.0855	0
9	HYB	1	HYB	C	aDC	-0.506500	12.0107	0
10	HYB	1	HYB	H	aDH	0.093940	1.0079	0
11	HYB	1	HYB	H	aDH	0.093940	1.0079	0
12	HYB	1	HYB	H	aDH	0.093940	1.0079	0
13	HYB	1	HYB	H	aDH	0.046500	1.0079	0
14	HYB	1	HYB	H	aDH	0.046500	1.0079	0
15	HYB	1	HYB	H	aDH	0.102300	1.0079	0
16	HYB	1	HYB	H	aDH	0.102300	1.0079	0
17	HYB	1	HYB	H	aDH	0.102300	1.0079	0
18	HYB	1	HYB	H	aDH	0.093940	1.0079	0
19	HYB	1	HYB	H	aDH	0.093940	1.0079	0
20	HYB	1	HYB	H	aDH	0.093940	1.0079	0
21	HYB	1	HYB	C	aDC	-0.506500	12.0107	0
22	HYB	1	HYB	H	aDH	0.093940	1.0079	0
23	HYB	1	HYB	H	aDH	0.093940	1.0079	0
24	HYB	1	HYB	H	aDH	0.093940	1.0079	0
25	HYB	1	HYB	C	aDC	-0.506500	12.0107	0
26	HYB	1	HYB	H	aDH	0.093940	1.0079	0
27	HYB	1	HYB	H	aDH	0.093940	1.0079	0
28	HYB	1	HYB	H	aDH	0.093940	1.0079	0
29	HYB	1	HYB	C	aDC	-0.506500	12.0107	0
30	HYB	1	HYB	H	aDH	0.093940	1.0079	0
31	HYB	1	HYB	H	aDH	0.093940	1.0079	0
32	HYB	1	HYB	H	aDH	0.093940	1.0079	0
33	HYB	1	HYB	C	aDC	-0.506500	12.0107	0
34	HYB	1	HYB	H	aDH	0.093940	1.0079	0
35	HYB	1	HYB	H	aDH	0.093940	1.0079	0
36	HYB	1	HYB	H	aDH	0.093940	1.0079	0
37	HYB	1	HYB	C	CCH2	0.014000	12.0107	0
38	HYB	1	HYB	C	CCH2	0.355000	12.0107	0
39	HYB	1	HYB	H	HCH2	-0.005000	1.0079	0
40	HYB	1	HYB	H	HCH2	-0.005000	1.0079	0
41	HYB	1	HYB	H	HCH2	-0.042000	1.0079	0
42	HYB	1	HYB	H	HCH2	-0.042000	1.0079	0
43	HYB	1	HYB	O	OPE	-0.528000	15.9994	0
44	HYB	1	HYB	C	CCH2	0.233000	12.0107	0
45	HYB	1	HYB	C	CCH2	0.441000	12.0107	0
46	HYB	1	HYB	H	HCH2	0.003500	1.0079	0
47	HYB	1	HYB	H	HCH2	0.003500	1.0079	0
48	HYB	1	HYB	H	HCH2	-0.039000	1.0079	0
49	HYB	1	HYB	H	HCH2	-0.039000	1.0079	0
50	HYB	1	HYB	O	OPE	-0.664000	15.9994	0
51	HYB	1	HYB	C	CCH2	0.344000	12.0107	0
52	HYB	1	HYB	C	CCH2	0.462000	12.0107	0

53	HYB	1	HYB	H	HCH2	-0.022500	1.0079	0
54	HYB	1	HYB	H	HCH2	-0.022500	1.0079	0
55	HYB	1	HYB	H	HCH2	-0.041500	1.0079	0
56	HYB	1	HYB	H	HCH2	-0.041500	1.0079	0
57	HYB	1	HYB	O	OPE	-0.670000	15.9994	0
58	HYB	1	HYB	C	CCH2	0.356000	12.0107	0
59	HYB	1	HYB	C	CCH2	0.308000	12.0107	0
60	HYB	1	HYB	H	HCH2	-0.029000	1.0079	0
61	HYB	1	HYB	H	HCH2	-0.029000	1.0079	0
62	HYB	1	HYB	H	HCH2	-0.000500	1.0079	0
63	HYB	1	HYB	H	HCH2	-0.000500	1.0079	0
64	HYB	1	HYB	O	OPE	-0.513000	15.9994	0
65	HYB	1	HYB	C	CCH3	0.199180	12.0107	0
66	HYB	1	HYB	H	HCH2	0.007000	1.0079	0
67	HYB	1	HYB	H	HCH2	0.007000	1.0079	0
68	HYB	1	HYB	H	HCH2	0.007000	1.0079	0

67 !NBOND: bonds

1	2	1	3	1	29	1	33
2	10	2	11	2	12	3	4
4	5	4	6	4	7	5	13
5	14	5	37	6	15	6	16
6	17	7	8	8	9	8	21
8	25	9	18	9	19	9	20
21	22	21	23	21	24	25	26
25	27	25	28	29	30	29	31
29	32	33	34	33	35	33	36
37	38	37	39	37	40	38	41
38	42	38	43	43	44	44	45
44	46	44	47	45	48	45	49
45	50	50	51	51	52	51	53
51	54	52	55	52	56	52	57
57	58	58	59	58	60	58	61
59	62	59	63	59	64	64	65
65	66	65	67	65	68		

126 !NTHETA: angles

2	1	3	2	1	29	2	1	33
1	2	10	1	2	11	1	2	12
3	1	29	3	1	33	1	3	4
29	1	33	1	29	30	1	29	31
1	29	32	1	33	34	1	33	35
1	33	36	10	2	11	10	2	12
11	2	12	3	4	5	3	4	6
3	4	7	5	4	6	5	4	7
4	5	13	4	5	14	4	5	37
6	4	7	4	6	15	4	6	16
4	6	17	4	7	8	13	5	14
13	5	37	14	5	37	5	37	38
5	37	39	5	37	40	15	6	16
15	6	17	16	6	17	7	8	9
7	8	21	7	8	25	9	8	21
9	8	25	8	9	18	8	9	19
8	9	20	21	8	25	8	21	22

8	21	23	8	21	24	8	25	26
8	25	27	8	25	28	18	9	19
18	9	20	19	9	20	22	21	23
22	21	24	23	21	24	26	25	27
26	25	28	27	25	28	30	29	31
30	29	32	31	29	32	34	33	35
34	33	36	35	33	36	38	37	39
38	37	40	37	38	41	37	38	42
37	38	43	39	37	40	41	38	42
41	38	43	42	38	43	38	43	44
43	44	45	43	44	46	43	44	47
45	44	46	45	44	47	44	45	48
44	45	49	44	45	50	46	44	47
48	45	49	48	45	50	49	45	50
45	50	51	50	51	52	50	51	53
50	51	54	52	51	53	52	51	54
51	52	55	51	52	56	51	52	57
53	51	54	55	52	56	55	52	57
56	52	57	52	57	58	57	58	59
57	58	60	57	58	61	59	58	60
59	58	61	58	59	62	58	59	63
58	59	64	60	58	61	62	59	63
62	59	64	63	59	64	59	64	65
64	65	66	64	65	67	64	65	68
66	65	67	66	65	68	67	65	68

153 !NPHI: dihedrals

3	1	2	10	3	1	2	11
3	1	2	12	2	1	3	4
29	1	2	10	29	1	2	11
29	1	2	12	2	1	29	30
2	1	29	31	2	1	29	32
33	1	2	10	33	1	2	11
33	1	2	12	2	1	33	34
2	1	33	35	2	1	33	36
29	1	3	4	3	1	29	30
3	1	29	31	3	1	29	32
33	1	3	4	3	1	33	34
3	1	33	35	3	1	33	36
1	3	4	5	1	3	4	6
1	3	4	7	33	1	29	30
33	1	29	31	33	1	29	32
29	1	33	34	29	1	33	35
29	1	33	36	3	4	5	13
3	4	5	14	3	4	5	37
3	4	6	15	3	4	6	16
3	4	6	17	3	4	7	8
6	4	5	13	6	4	5	14
6	4	5	37	5	4	6	15
5	4	6	16	5	4	6	17
7	4	5	13	7	4	5	14
7	4	5	37	5	4	7	8
4	5	37	38	4	5	37	39
4	5	37	40	7	4	6	15

7	4	6	16	7	4	6	17
6	4	7	8	4	7	8	9
4	7	8	21	4	7	8	25
13	5	37	38	13	5	37	39
13	5	37	40	14	5	37	38
14	5	37	39	14	5	37	40
5	37	38	41	5	37	38	42
5	37	38	43	7	8	9	18
7	8	9	19	7	8	9	20
7	8	21	22	7	8	21	23
7	8	21	24	7	8	25	26
7	8	25	27	7	8	25	28
21	8	9	18	21	8	9	19
21	8	9	20	9	8	21	22
9	8	21	23	9	8	21	24
25	8	9	18	25	8	9	19
25	8	9	20	9	8	25	26
9	8	25	27	9	8	25	28
25	8	21	22	25	8	21	23
25	8	21	24	21	8	25	26
21	8	25	27	21	8	25	28
39	37	38	41	39	37	38	42
39	37	38	43	40	37	38	41
40	37	38	42	40	37	38	43
37	38	43	44	41	38	43	44
42	38	43	44	38	43	44	45
38	43	44	46	38	43	44	47
43	44	45	48	43	44	45	49
43	44	45	50	46	44	45	48
46	44	45	49	46	44	45	50
47	44	45	48	47	44	45	49
47	44	45	50	44	45	50	51
48	45	50	51	49	45	50	51
45	50	51	52	45	50	51	53
45	50	51	54	50	51	52	55
50	51	52	56	50	51	52	57
53	51	52	55	53	51	52	56
53	51	52	57	54	51	52	55
54	51	52	56	54	51	52	57
51	52	57	58	55	52	57	58
56	52	57	58	52	57	58	59
52	57	58	60	52	57	58	61
57	58	59	62	57	58	59	63
57	58	59	64	60	58	59	62
60	58	59	63	60	58	59	64
61	58	59	62	61	58	59	63
61	58	59	64	58	59	64	65
62	59	64	65	63	59	64	65
59	64	65	66	59	64	65	67
59	64	65	68				

0 !NIMPHI: impropers

The classical FF parameters for the PEGS molecule is given below. It includes the force field parameters for different types of bonds, angles, dihedrals, impropers, and van der Waals potentials.

```
BONDS
!
!V(bond) = Kb(b - b0)**2
!
!Kb: kcal/mole/Ang**2
!b0: Ang
!
!atom type Kb b0
!
! Bonds for 1-ethyl-3-MeImid+
!
aDSI aDO 350.0 1.653
aDSI aDC 190.0 1.881
aDC aDH 328.0 1.095
aDC CCH2 268.0 1.538
CCH2 CCH2 268.0 1.521
CCH2 HCH2 340.0 1.099
CCH3 HCH2 340.0 1.096
CCH2 OPE 320.0 1.417
CCH3 OPE 320.0 1.414
!
!
ANGLES
!
!V(angle) = Ktheta(Theta - Theta0)**2
!
!Ktheta: kcal/mole/rad**2
!Theta0: degrees
!
!atom types Ktheta Theta0
!
! Angles for 1-Butyl-3-MeImid+
!
aDSI aDO aDSI 14.149 144.0
aDO aDSI aDO 94.551 109.5
aDO aDSI aDC 50.000 109.5
aDC aDSI aDC 50.000 109.5
aDSI aDC aDH 28.770 111.09
aDH aDC aDH 38.50 107.77
aDSI aDC CCH2 58.350 115.66
aDH aDC CCH2 26.50 109.37
aDC CCH2 HCH2 26.50 110.24
aDC CCH2 CCH2 58.350 113.77
CCH2 CCH2 HCH2 37.5 109.64
HCH2 CCH2 HCH2 33.0 107.75
HCH2 CCH3 HCH2 33.0 108.91
CCH2 CCH2 OPE 50.0 107.89
OPE CCH2 HCH2 35.0 110.63
OPE CCH3 HCH2 35.0 110.01
CCH2 OPE CCH2 60.0 113.42
CCH2 OPE CCH3 60.0 113.06
!
!
```

```
!
DIHEDRALS
!
!V(dihedral) = Kchi(1 + cos(n(chi) - delta))
!
!Kchi: kcal/mole
!n: multiplicity
!delta: degrees
!
!atom types Kchi n delta
!
aDSI aDO aDSI aDO 0.225 1 0.0000
aDSI aDO aDSI aDC 0.01 3 0.0000
aDO aDSI aDC aDH 0.075 3 0.0000
aDC aDSI aDC aDH 0.075 3 0.0000
aDO aDSI aDC CCH2 0.3527 1 0.0000
aDO aDSI aDC CCH2 -0.0677 2 180.00
aDO aDSI aDC CCH2 0.7862 3 0.0000
aDC aDSI aDC CCH2 0.3527 1 0.0000
aDC aDSI aDC CCH2 -0.0677 2 180.00
aDC aDSI aDC CCH2 0.7862 3 0.0000
aDSI aDC CCH2 CCH2 0.7054 1 0.0000
aDSI aDC CCH2 CCH2 -0.1355 2 180.00
aDSI aDC CCH2 CCH2 1.5724 3 0.0000
aDSI aDC CCH2 HCH2 0.1950 3 0.0000
aDC CCH2 CCH2 OPE 0.1600 1 180.00
aDC CCH2 CCH2 OPE 0.3900 2 0.00
aDC CCH2 CCH2 HCH2 0.1950 3 0.0000
CCH2 CCH2 aDC aDH 0.1950 3 0.0000
aDH aDC CCH2 HCH2 0.1591 3 0.0000
HCH2 CCH2 CCH2 HCH2 0.1591 3 0.0000
HCH2 CCH2 CCH2 OPE 0.234 3 0.0000
CCH2 OPE CCH2 HCH2 0.38 3 0.00
CCH2 OPE CCH3 HCH2 0.38 3 0.00
CCH3 OPE CCH2 HCH2 0.38 3 0.00
CCH2 OPE CCH2 CCH2 0.834 1 0.00
CCH2 OPE CCH2 CCH2 -0.283 2 180.0
CCH2 OPE CCH2 CCH2 -0.00165 3 0.00
CCH2 OPE CCH2 CCH2 -0.1466 4 180.0
CCH3 OPE CCH2 CCH2 0.834 1 0.00
CCH3 OPE CCH2 CCH2 -0.283 2 180.0
CCH3 OPE CCH2 CCH2 -0.00165 3 0.00
CCH3 OPE CCH2 CCH2 -0.1466 4 180.0
OPE CCH2 CCH2 OPE 1.4108 1 0.00
OPE CCH2 CCH2 OPE -1.2811 2 180.0
OPE CCH2 CCH2 OPE 0.4110 3 0.00
OPE CCH2 CCH2 OPE -0.4604 4 180.0
!
!
!
!V(Lennard-Jones) = Eps,i,j[(Rmin,i,j/ri,j)**12 - 2(Rmin,i,j/ri,j)**6]
!
!epsilon: kcal/mole, Eps,i,j = sqrt(eps,i * eps,j)
!Rmin/2: A, Rmin,i,j = Rmin/2,i + Rmin/2,j
```

```
!
!atom ignored epsilon Rmin/2 ignored eps,1-4 Rmin/2,1-4
!
!
!
aDSI 0.000000 -0.2381 2.0885707458 0.0000 -0.119050 2.0885707458
aDC 0.000000 -0.08076 1.8585446022 0.0000 -0.040380 1.8585446022
aDO 0.000000 -0.19970 1.5640666866 0.0000 -0.099850 1.5640666866
aDH 0.000000 -0.00915 1.47213      0.0000 -0.004575 1.47213
CCH2 0.00000 -0.066   1.94466549915 0.0000 -0.033 1.94466549915
CCH3 0.00000 -0.066 1.94466549915 0.0000  -0.033  1.94466549915
HCH2 0.000000 -0.03 1.38904678539 0.0000 -0.015   1.38904678539
OPE 0.000000 -0.14  1.6112942802  0.0000 -0.07    1.6112942802
!
END
```

2 Validation of the In-house Software to Compute Viscosity

To confirm viscosity calculations by using the locally developed software, a flexible SPC/Fw water model[1] was used to calculate the water viscosity at 298 K and 1 bar. The simulation box contains 600 water molecules and 10-ns NVE MD production runs were implemented by following the NPT and NVT runs. Simulation time step was set to be 0.5 fs. Pressure tensors were saved every 0.5 fs. All MD simulations were performed by using the NAMD program.[2] When the Green-Kubo method was used, the whole 10-ns NVE runs were divided into five blocks. For each block, viscosity was calculated in the following manner. Integration of $\langle P_{\zeta\nu}(t)P_{\zeta\nu}(0)\rangle$ was performed over a short time period of 10 ps; viscosity was calculated by fitting to the integration values over this 10-ps time period. The final viscosity was calculated by averaging the viscosity values for those five different blocks and it was calculated to be $0.77 \pm 0.04 \times 10^{-3}$ Pa.s. When the Einstein method was used, the whole 10-ns NVE runs were not divided into separate blocks and they were used to obtain a single $A(t)$. The $A(t)$ values between 255-370 ps were then used to calculate the viscosity. Note that in this time period it was found that $\beta = 1.02 \pm 0.01$. The Einstein method gives a viscosity value of $0.72 \pm 0.01 \times 10^{-3}$ Pa.s. The Einstein and Green-Kubo methods give consistent water viscosity values, both of which agree reasonably well with the simulation value of $0.886 \pm 0.142 \times 10^{-3}$ Pa.s obtained by Raabe *et al.* from NVT MD simulations.[3] The small viscosity difference between this work and Raabe is partly due to the fact that NVE simulations were used in this work to obtain the viscosity. Indeed, our calculations (not shown here) indicate that NVT simulation gives a larger viscosity compared to the NVE simulation. We used the NVE simulation in transport property calculation to avoid velocity perturbation due to the temperature control in NVT simulations. Additionally, we have also calculated the viscosity for liquid n-decane at 298 K. Our simulated viscosity values are $0.56 \pm 0.15 \times 10^{-3}$ Pa.s (Green-Kubo) and $0.57 \pm 0.01 \times 10^{-3}$ Pa.s (Einstein method), both of which agree with each

other and they are close to the simulated value of $0.67 \pm 0.04 \times 10^{-3}$ Pa.s obtained by Mondello *et al.* from NVT simulation.[4] As expected, our simulated viscosity values for n-decane from NVE simulations are slightly smaller than the value obtained by Mondello *et al.* from NVT simulation. The viscosity agreement for water and n-decane between our calculations and other groups indicates that we have correctly implemented viscosity calculation by using the in-house software.

3 Validation of the Procedure to Compute Heat Capacity

In order to confirm the procedure to calculate heat capacity, the heat capacities for liquid water and liquid benzene were calculated. The ideal gas heat capacity ($C^{\mathrm{ig}}_{\mathrm{P,m}}$) values for water at 298-370 K were calculated to be 33.48-33.90 J/(mol.K) from quantum calculations at the B3LYP/6-311++G(d,p) level of theory. The $C^{\mathrm{ig}}_{\mathrm{P,m}}$ values are very close to the experimental data,[5] with a small difference of 0.3%. By using a higher level theory of MP2/aug-cc-pVTZ for both geometry optimization and frequency calculations, the water $C^{\mathrm{ig}}_{\mathrm{P,m}}$ values were found to change only slightly by 0.03 J/(mol.K) compared to the B3LYP/6-311++G(d,p) method. These findings suggest that quantum AI calculations could accurately predict $C^{\mathrm{ig}}_{\mathrm{P,m}}$. By adding $C^{\mathrm{res}}_{\mathrm{P,m}}$ to $C^{\mathrm{ig}}_{\mathrm{P,m}}$, the total liquid water heat capacity ($C_{\mathrm{P,m}}$) values at 298-370 K and 1 bar were calculated to be 89.4-89.8 J/(mol.K) by using a flexible SPC water model.[6] These simulated $C_{\mathrm{P,m}}$ values for water are 19% larger than the experimental data.[7] For benzene, by using the B3LYP/6-311++G(d,p) method the $C^{\mathrm{ig}}_{\mathrm{P,m}}$ values at 273-370 K were calculated to be $72.75-102.17$ J/(mol.K), which are also close to the experimental data,[5] with a small difference of 2-3%. The $C^{\mathrm{ig}}_{\mathrm{P,m}}$ difference is small (1-2 J/(mol.K)) between the B3LYP/6-311++G(d,p) and MP2/aug-cc-pVTZ methods. The total liquid benzene heat capacity values at 298-340 K were calculated to be 141-152 J/(mol.K) by using an atomistic benzene model.[8] The simulated benzene $C_{\mathrm{P,m}}$ values are 6-7% larger than the experimental

data.[7] The reasonable agreement in $C^{\mathrm{ig}}_{\mathrm{P,m}}$ and $C_{\mathrm{P,m}}$ between simulations and experiments suggest that we have correctly implemented heat capacity calculations.

4 RI-MP2 Quantum Calculations

A series of structures were created in order to assess the accuracy of the classical force field by comparison with ab initio interaction energies. The quantity of interest in this case is the interaction energy between the gas molecule and the PEMS molecule. The interaction energies were calculated for 5-6 structures for each of the four gases, namely: CO_2-PEGS, H_2-PEGS, H_2S-PEGS, and H_2O-PEGS. For each of the 22 structures, the interaction energy was calculated at the RI-MP2[9–11] level with the cc-pVDZ, cc-pVTZ, and cc-pVQZ basis sets.[12] The results were extrapolated to the complete basis set limit using the following expression,[13] $E_{\mathrm{int(n)}} = E_{\mathrm{int(CBS)}} + Ae^{-Bx}$, where $E_{\mathrm{int(n)}}$ is the interaction energy calculated with basis set n, and $E_{\mathrm{int}(CBS)}$ is the interaction energy extrapolated to the complete basis set limit. The calculations were carried out with the Q-Chem ab initio program.[14]

In Figure S2, the interaction energies yielded by the force field are plotted against the ab initio energies. While agreement is reasonably good for the CO_2-PEGS and H_2-PEGS interaction energies, the force field tends to slightly underestimate the H_2S-PEGS interactions and to overestimate the H_2O-PEGS interactions.

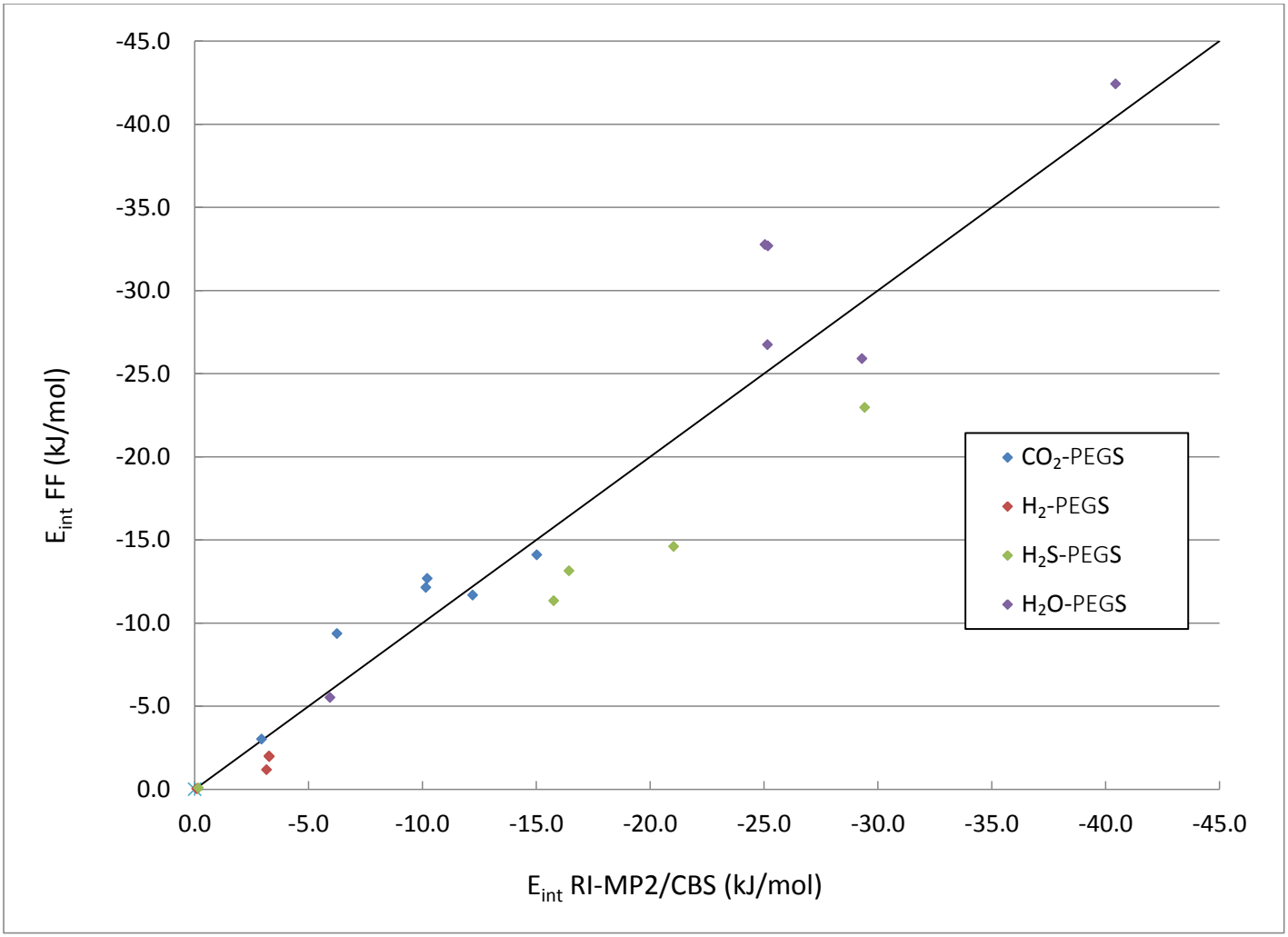

Figure S2: CO_2, H_2, H_2S, and H_2O interactions with the PEGS molecule obtained from classcial force field (FF) and quantum RI-MP2 calculations.

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