Supporting Information

Gaussian-Charge Polarizable and Non-Polarizable Models for CO_2

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Table 1: Saturated density (in kg/m^3) of CO_2 calculated from the proposed polarizable and non-polarizable models. Statistical uncertainties are given in parentheses in units of the last significant figure shown: 1055(2) means 1055±2.

T (K)	Polarizable model		Non-polarizable model	
	ρ_L	ρ_v	ρ_L	ρ_v
220	1155(2)	16.6(8)	1162.3(8)	16.49(8)
230	1119(2)	25.5(6)	1126.3(7)	24.26(9)
240	1084(3)	33.7(9)	1088.9(7)	33.9(1)
250	1044(3)	48(1)	1049.3(9)	46.8(2)
260	997(3)	67(1)	1006(1)	64.8(3)
270	948(3)	89(2)	957(1)	88.2(4)
280	879(4)	119(3)	898(2)	118.6(3)
290	820(4)	176(4)	828(2)	163.7(8)

Table 2: Saturated vapor pressure (in bar) of CO_2 calculated from the proposed polarizable and non-polarizable models. Statistical uncertainties are given as in Table 1.

T (K)	Polarizable model	Non-polarizable model
220	6.3(2)	6.2(1)
230	9.6(3)	9.4(1)
240	13.3(4)	13.3(1)
250	18.2(5)	18.3(2)
260	25.6(5)	25.0(2)
270	32.6(4)	33.0(2)
280	41.7(5)	42.3(3)
290	54.1(7)	53.8(3)

Table 3: Enthalpy of vaporization (in kJ/mol) of CO_2 calculated from the proposed polarizable and non-polarizable models. Statistical uncertainties are given as in Table 1.

T (K)	Polarizable model	Non-polarizable model
220	14.79(7)	15.00(5)
230	14.08(4)	14.30(4)
240	13.55(6)	13.57(5)
250	12.56(8)	12.75(7)
260	11.68(7)	11.82(5)
270	10.7(1)	10.78(8)
280	9.1(2)	9.49(9)
290	7.6(2)	7.9(1)

Table 4: Second virial coefficient (in L/mol) of CO_2 calculated from the proposed polarizable and non-polarizable models. Statistical uncertainties are given as in Table 1.

T (K)	Polarizable model	Non-polarizable model
220	-0.2144	-0.2150
230	-0.1942	-0.1952
240	-0.1771	-0.1779
250	-0.1621	-0.1628
260	-0.1489	-0.1494
270	-0.1372	-0.1376
280	-0.1267	-0.1271
290	-0.1172	-0.1175
300	-0.1087	-0.1089
350	-0.076	-0.0761
400	-0.0539	-0.0539
450	-0.0382	-0.0382
500	-0.0264	-0.0263
600	-0.0100	-0.0099
700	0.0007	0.0009
800	0.0083	0.0085
900	0.0139	0.0141
1000	0.0182	0.0183
1200	0.0242	0.0244

Table 5: Liquid density (in kg/m^3) of CO_2 calculated from the proposed polarizable and non-polarizable models. Statistical uncertainties are given as in Table 1.

T (K)	P (bar)	Polarizable model	Non-polarizable model
250	50	1051.8(7)	1061.3(2)
300	50	121.2(8)	122.1(6)
400	50	71.9(1)	72.12 (4)
500	50	54.4(2)	54.55(2)
600	50	44.3(1)	44.4(1)
250	100	1069.5(4)	1077.1(1)
300	100	808(3)	821.1(4)
350	100	218(1)	220.5(3)
400	100	158.5(3)	158.8(1)
500	100	111.9(3)	112.28(4)
600	100	89.4(2)	89.6(1)
250	1000	1219.7(3)	1226.1(1)
300	1000	1117.9(3)	1123.8(1)
350	1000	1019.3(6)	1020.0(4)
400	1000	926.6(7)	930.6(2)
500	1000	766.4(6)	768.3(2)
600	1000	645.9(4)	646.7(1)
300	2000	1227.2(3)	1232.6(1)
350	2000	1154.4(1)	1159.4(1)
400	2000	1087.7(4)	1091.6(1)
500	2000	968.9(3)	971.8(1)
600	2000	870.3(3)	872.5(1)

Table 6: Isobaric heat capacity of CO_2 at 100 bar (in J/mol/K) calculated from the proposed polarizable and non-polarizable models. Statistical uncertainties are given as in Table 1.

T (K)	Polarizable model	Non-polarizable model
220	80.4(6)	79(1)
250	81.5(7)	80(1)
275	92(2)	90(2)
300	124(4)	128(5)
310	195(4)	190(4)
320	376(14)	424(12)
330	132(6)	138(4)
340	94(4)	89(3)
350	78(2)	74(5)
400	52(2)	54(1)
500	49(2)	49(2)
600	48(2)	48(1)
700	50(2)	50(2)
800	51(2)	51(2)

Table 7: Isochoric capacity of CO_2 at 50 bar (in J/mol/K) calculated from the proposed polarizable and non-polarizable models. Statistical uncertainties are given as in Table 1.

T (K)	Polarizable model	Non-polarizable model
220	38.9(4)	39.2(4)
230	38.1(7)	38.1(8)
240	37.8(7)	35.7(7)
250	36.9(8)	35.9(7)
260	36.6(8)	36.3(8)
270	36.5(9)	35.5(9)
280	36(1)	35(1)
290	34.7(9)	36(1)
300	31(1)	32(1)
350	31(1)	31(1)
400	29.8(8)	32(1)
500	32(3)	35(3)
600	37(2)	35(2)
800	43(3)	41(3)
1000	46(2)	47(3)

Table 8: Self-diffusion coefficients (in $10^{-9}m^2/s$) of the proposed polarizable and non-polarizable CO_2 models for various temperatures and pressures.

T (K)	P (MPa)	Polarizable model	Non-polarizable model
223	10	4.95(9)	4.99(8)
233	20	4.7(2)	4.70(8)
223	50	4.1(1)	4.1(1)
223	100	3.25(7)	3.4(1)
298	10	19.5(6)	18.7(6)
298	20	15.0(4)	15.3(4)
298	100	8.8(2)	9.0(2)
298	200	6.2(1)	6.5(1)
373	50	24.2(5)	24.6(8)
373	100	16.4(4)	16.4(3)
373	150	13.1(2)	13.2(4)
373	200	10.9(2)	11.1(3)
450	100	27.0(7)	27.2(4)
450	150	20.8(4)	21.1(6)
450	200	17.4(4)	17.5(4)

Table 9: Viscosity (in cP) of the proposed polarizable and non-polarizable CO_2 models for various temperatures and pressures.

T (K)	P (MPa)	Polarizable model	Non-polarizable model
273	10	0.127(3)	0.123(1)
273	50	0.187(5)	0.182(2)
273	100	0.250(2)	0.242(5)
273	200	0.345(7)	0.35(1)
323	10	0.0272(4)	0.076(2)
323	50	0.123(2)	0.114(2)
323	100	0.171(2)	0.168(3)
323	200	0.25(1)	0.250(5)
373	20	0.037(1)	0.037(2)
373	50	0.082(1)	0.0834(1)
373	100	0.127(2)	0.1229(2)
373	200	0.189(4)	0.1961(1)
423	20	0.03(1)	0.031(1)
423	50	0.06(1)	0.061(3)
423	100	0.099(1)	0.100(4)
423	200	0159(1)	0.156(3)

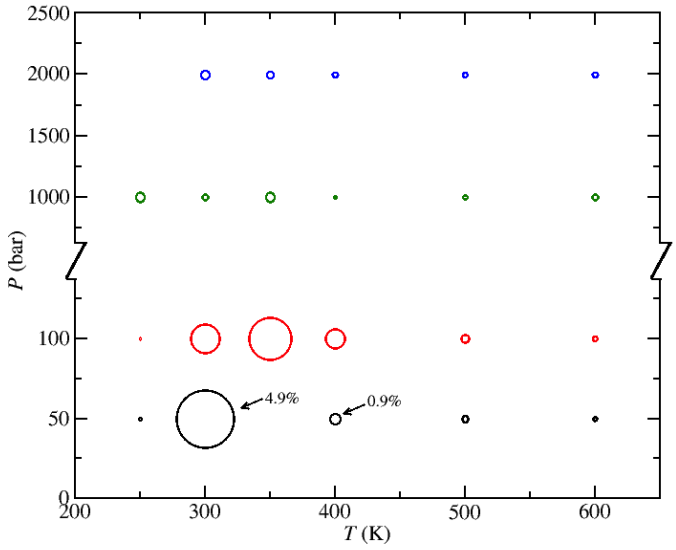

Figure 1: Relative deviations for density in one-phase fluid region between the non-polarizable model calculation and experimental data from NIST. The size of circles is proportional to the relative deviation.

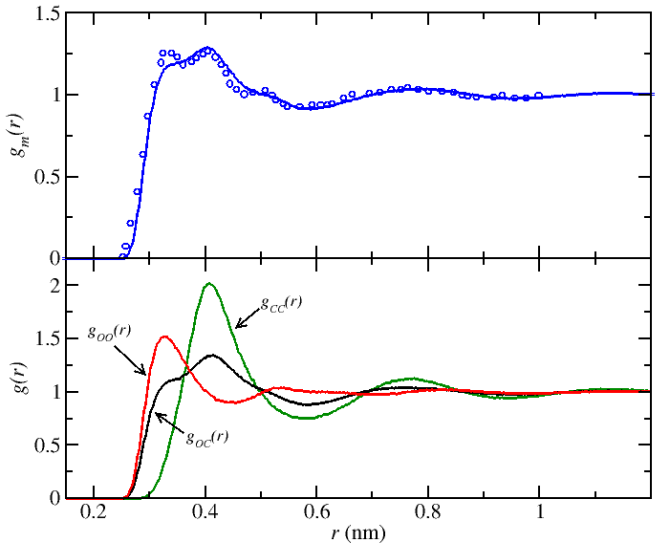

Figure 2: Atom-atom radial distribution functions of the non-polarizable CO_2 model (bottom) and neutron weighted pair correlation function $g_N(r)$ (top) at 239 K and 14.5 bar. Experimental pair correlation function is shown as blue circles, and the simulation results from the non-polarizable model are shown as solid lines.

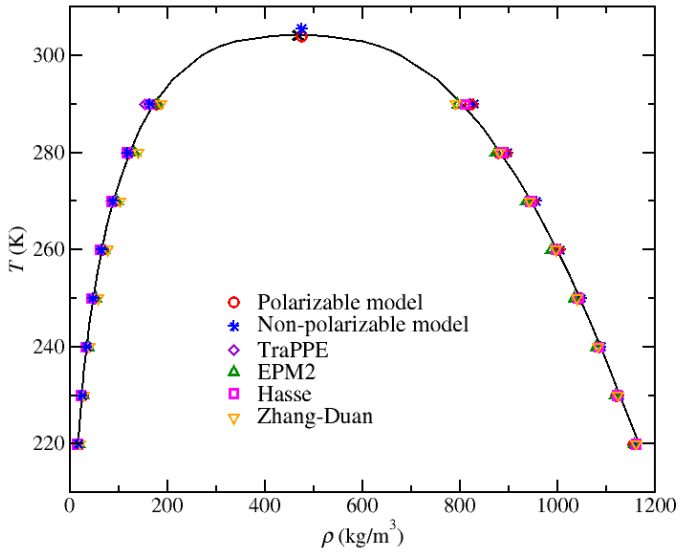

Figure 3: Vapor-liquid coexistence curve calculated from proposed polarizable, non-polarizable, TraPPE, EPM2, Hasse and Zhang-Duan models from 220 K to 290 K. Solid line is experimental data from NIST.

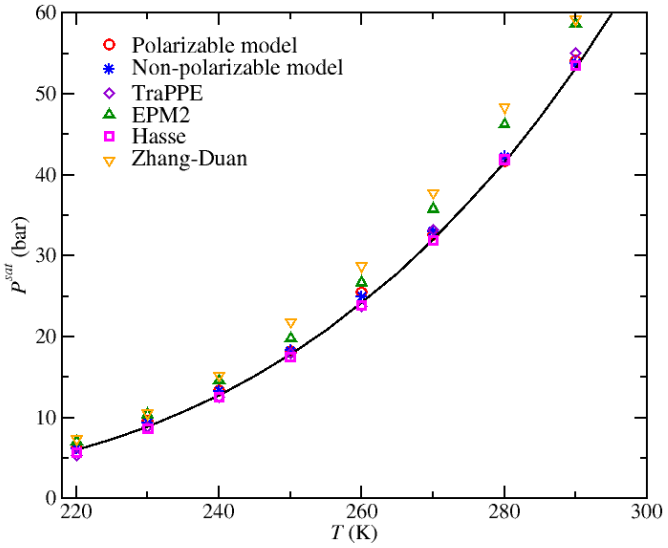

Figure 4: Saturated vapor pressure calculated from proposed polarizable, non-polarizable, TraPPE, EPM2, Hasse and Zhang-Duan models from 220 K to 290 K. Solid line is experimental data from NIST.

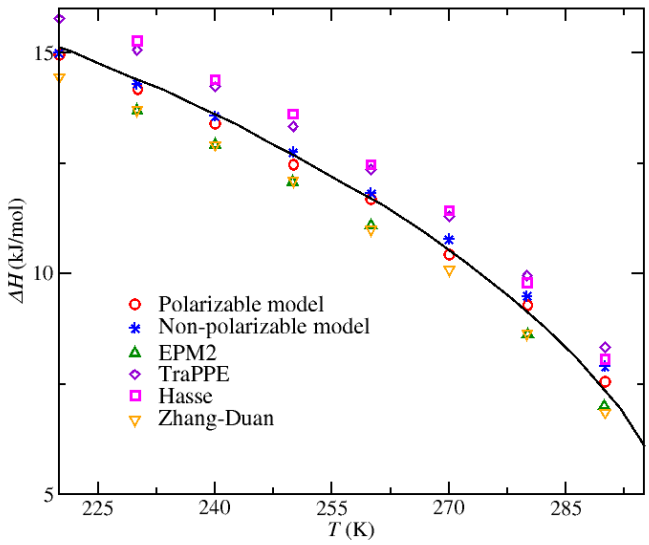

Figure 5: Enthalpy of vaporization calculated from proposed polarizable, non-polarizable, TraPPE, EPM2, Hasse and Zhang-Duan models from 220 K to 290 K. Solid line is experimental data from NIST.

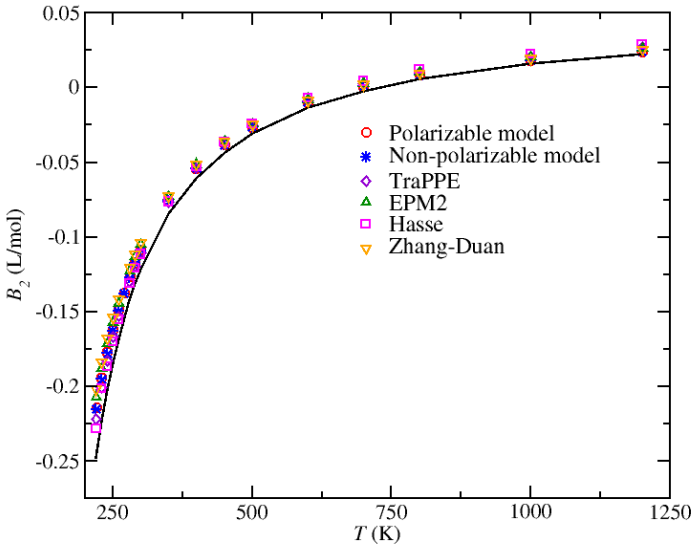

Figure 6: Second virial coefficients calculated from proposed polarizable, non-polarizable, TraPPE, EPM2, Hasse and Zhang-Duan models from 220 K to 1200 K. Solid line is experimental data from NIST.

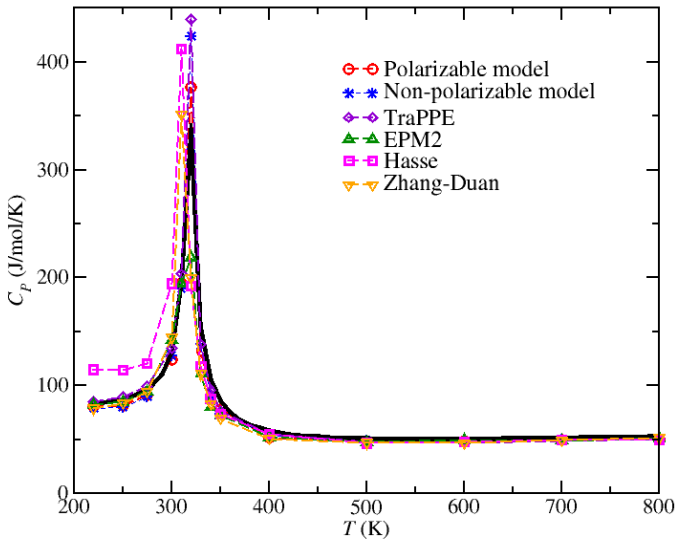

Figure 7: Isobaric heat at 100 bar capacity calculated from proposed polarizable, non-polarizable, TraPPE, EPM2, Hasse and Zhang-Duan models. Solid line is experimental data from NIST.

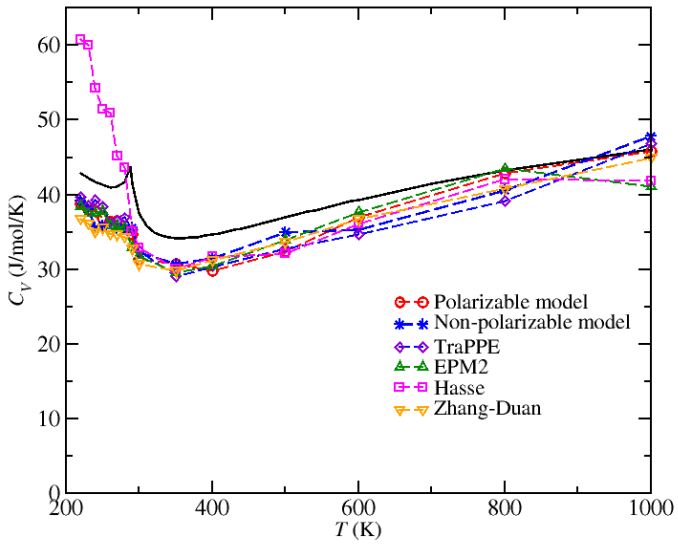

Figure 8: Isochoric heat capacity at 50 bar calculated from proposed polarizable, non-polarizable, TraPPE, EPM2, Hasse and Zhang-Duan models. Solid line is experimental data from NIST.

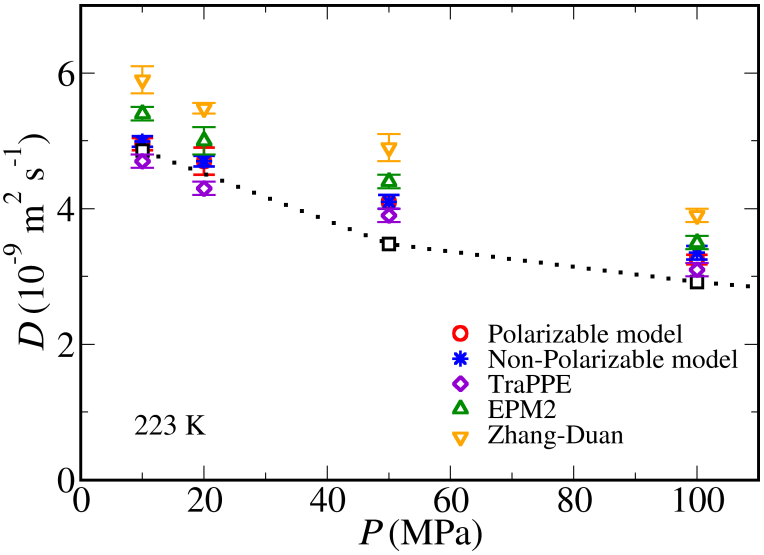

Figure 9: Self-diffusion coefficient at 223 K calculated from proposed polarizable, non-polarizable, TraPPE, EPM2 and Zhang-Duan models. Black open squares are the experimental data by Grob *et al.*, and the dotted line is to guide the eye.

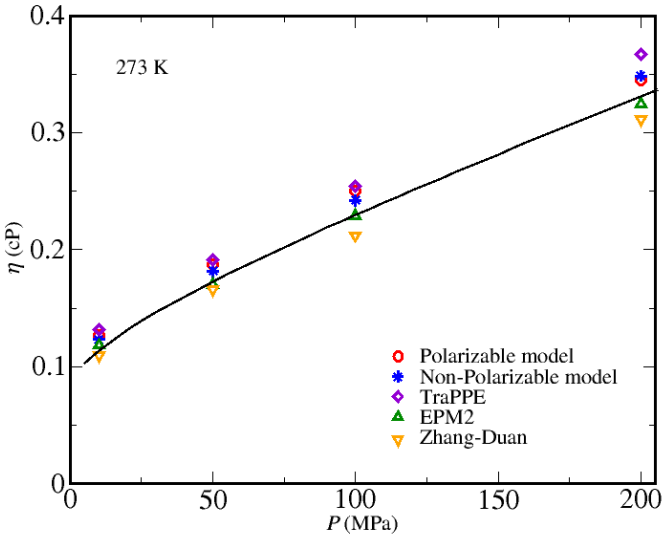

Figure 10: Viscosity at 273 K calculated from proposed polarizable, non-polarizable, TraPPE, EPM2 and Zhang-Duan models. Solid line is experimental data from Groß *et al.*