

## Supporting Information

### Molecular Simulation of Thermodynamic and Transport Properties for the H<sub>2</sub>O+NaCl System

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Table 1: Simulation results for the vapor pressure,  $P^{\text{sat}}$ , of different model combinations at  $T = 298$  K. Statistical uncertainties are given in parentheses in units of the last significant figure shown: 0.031(4) means  $0.031 \pm 0.004$ .

| $m$<br>(mol/kg) | $P^{\text{sat}}$ (bar) |          |          |
|-----------------|------------------------|----------|----------|
|                 | SPC+JC                 | SPC+SD   | Exp6+TF  |
| 1.0             | 0.031(4)               | 0.031(3) | 0.033(3) |
| 2.0             | 0.031(4)               | 0.030(4) | 0.036(3) |
| 3.0             | 0.028(4)               | 0.029(4) | 0.034(3) |
| 4.0             | 0.027(3)               | 0.028(4) | 0.033(4) |

Table 2: Simulation results for the vapor pressure,  $P^{\text{sat}}$ , of different model combinations at  $T = 373$  K. Statistical uncertainties are given as in Table 1.

| $m$<br>(mol/kg) | $P^{\text{sat}}$ (bar) |         |              |              |                       |                       |         |
|-----------------|------------------------|---------|--------------|--------------|-----------------------|-----------------------|---------|
|                 | SPC+JC                 | SPC+SD  | SPC/E<br>+JC | SPC/E<br>+SD | Semiflex.<br>SPC/E+JC | Semiflex.<br>SPC/E+SD | Exp6+TF |
| 0.10            | 1.13(4)                | 1.16(5) | 0.41(2)      | 0.41(3)      | 0.26(2)               | 0.28(4)               | 1.14(4) |
| 0.41            | 1.12(4)                | 1.12(5) | 0.40(2)      | 0.42(3)      | 0.24(2)               | 0.25(2)               | –       |
| 0.42            | –                      | –       | –            | –            | –                     | –                     | 1.13(2) |
| 0.92            | 1.11(5)                | 1.09(4) | 0.40(3)      | 0.40(2)      | 0.26(3)               | 0.27(3)               | –       |
| 0.94            | –                      | –       | –            | –            | –                     | –                     | 1.12(5) |
| 1.53            | 1.04(5)                | 1.12(5) | 0.41(4)      | 0.40(2)      | 0.24(2)               | 0.23(2)               | –       |
| 1.56            | –                      | –       | –            | –            | –                     | –                     | 1.04(5) |
| 2.76            | 1.00(5)                | 1.02(5) | –            | 0.36(3)      | 0.24(4)               | 0.24(3)               | –       |
| 2.80            | –                      | –       | –            | –            | –                     | –                     | 1.00(5) |
| 3.66            | 1.02(4)                | 1.01(5) | 0.36(2)      | 0.37(2)      | 0.22(2)               | 0.21(3)               | –       |
| 3.74            | –                      | –       | –            | –            | –                     | –                     | 1.02(4) |
| 4.37            | 0.95(5)                | 0.98(4) | 0.34(2)      | 0.35(3)      | 0.21(2)               | 0.22(2)               | –       |
| 4.46            | –                      | –       | –            | –            | –                     | –                     | 0.95(5) |
| 5.49            | 0.88(5)                | 0.99(7) | 0.30(3)      | –            | 0.19(3)               | 0.22(2)               | –       |
| 5.61            | –                      | –       | –            | –            | –                     | –                     | 0.88(6) |

Table 3: Simulation results for the vapor pressure,  $P^{\text{sat}}$ , of different model combinations at  $T = 473\text{K}$ . Statistical uncertainties are given as in Table 1.

| $m$<br>(mol/kg) | $P^{\text{sat}}$ (bar) |         |              |              |                       |                       |         |
|-----------------|------------------------|---------|--------------|--------------|-----------------------|-----------------------|---------|
|                 | SPC+JC                 | SPC+SD  | SPC/E<br>+JC | SPC/E<br>+SD | Semiflex.<br>SPC/E+JC | Semiflex.<br>SPC/E+SD | Exp6+TF |
| 0.12            | –                      | –       | –            | –            | 5.9(1)                | 5.8(2)                | –       |
| 0.14            | –                      | –       | 8.8(3)       | 8.9(2)       | –                     | –                     | –       |
| 0.16            | –                      | –       | –            | –            | –                     | –                     | 15.8(2) |
| 0.30            | –                      | 18.3(4) | –            | –            | –                     | –                     | –       |
| 0.31            | 18.3(4)                | –       | –            | –            | –                     | –                     | –       |
| 0.50            | –                      | –       | –            | –            | 5.9(1)                | 6.0(2)                | –       |
| 0.54            | –                      | –       | 8.6(3)       | –            | –                     | –                     | –       |
| 0.56            | –                      | –       | –            | 8.4(3)       | –                     | –                     | –       |
| 0.64            | –                      | –       | –            | –            | –                     | –                     | 15.7(2) |
| 1.08            | –                      | 17.3(4) | –            | –            | –                     | –                     | –       |
| 1.11            | –                      | –       | –            | –            | 5.7(3)                | 5.9(2)                | –       |
| 1.14            | 17.3(4)                | –       | –            | –            | –                     | –                     | –       |
| 1.18            | –                      | –       | 8.5(3)       | –            | –                     | –                     | –       |
| 1.26            | –                      | –       | –            | 8.5(2)       | –                     | –                     | –       |
| 1.43            | –                      | –       | –            | –            | –                     | –                     | 15.6(2) |
| 1.82            | –                      | –       | –            | –            | 5.6(2)                | 5.8(3)                | –       |
| 1.84            | –                      | –       | 8.2(2)       | –            | –                     | –                     | –       |
| 2.09            | –                      | –       | –            | 8.4(3)       | –                     | –                     | –       |
| 2.16            | 17.1(3)                | –       | –            | –            | –                     | –                     | –       |
| 2.32            | –                      | 17.1(4) | –            | –            | –                     | –                     | –       |
| 2.43            | –                      | –       | –            | –            | –                     | –                     | 15.9(4) |
| 2.99            | –                      | –       | 7.7(3)       | –            | –                     | –                     | –       |
| 3.22            | –                      | –       | –            | –            | 5.0(2)                | 5.3(2)                | –       |
| 3.66            | –                      | –       | –            | 7.9(3)       | –                     | –                     | –       |
| 3.71            | –                      | –       | 7.2(4)       | –            | –                     | –                     | –       |
| 3.74            | 16.9(5)                | –       | –            | –            | –                     | –                     | –       |
| 3.77            | –                      | 16.9(3) | –            | –            | –                     | –                     | –       |
| 4.29            | –                      | –       | –            | –            | 5.0(2)                | 5.3(2)                | –       |
| 4.30            | –                      | –       | –            | –            | –                     | –                     | 15.6(4) |
| 4.81            | –                      | –       | –            | 7.6(2)       | –                     | –                     | –       |
| 4.95            | –                      | –       | 6.9(3)       | –            | –                     | –                     | –       |
| 5.10            | –                      | –       | –            | –            | 4.7(2)                | 5.2(3)                | –       |
| 5.70            | 15.9(5)                | –       | –            | –            | –                     | –                     | –       |
| 5.72            | –                      | –       | –            | –            | –                     | –                     | 15.5(4) |
| 5.74            | –                      | –       | –            | 7.6(2)       | –                     | –                     | –       |
| 6.07            | –                      | 15.9(3) | –            | –            | –                     | –                     | –       |

Table 4: Simulation results for the density,  $\rho$ , of different model combinations. Statistical uncertainties are given as in Table 1.

| P<br>(bar) | T<br>(K) | $m$<br>(mol/kg) | $\rho$ (kg/m <sup>3</sup> ) |                       |                       |         |
|------------|----------|-----------------|-----------------------------|-----------------------|-----------------------|---------|
|            |          |                 | SPC/E+JC                    | Semiflex.<br>SPC/E+JC | Semiflex.<br>SPC/E+SD | Exp6+TF |
| 100        | 298      | 1.0             | 1046(2)                     | 1057(1)               | 1054(1)               | 1051(3) |
|            |          | 2.0             | 1069(3)                     | 1095(1)               | 1087(1)               | 1087(4) |
|            |          | 3.0             | 1103(2)                     | 1129(1)               | 1116(1)               | 1114(3) |
|            |          | 4.0             | 1139(3)                     | 1159(1)               | 1143(1)               | 1149(2) |
| 100        | 373      | 1.0             | 994(2)                      | 1003(3)               | 1001(3)               | 987(1)  |
|            |          | 2.0             | 1031(3)                     | –                     | –                     | –       |
|            |          | 3.0             | 1067(3)                     | 1073(4)               | 1062(4)               | 1053(2) |
|            |          | 4.0             | –                           | 1104(4)               | 1088(2)               | 1080(2) |
|            |          | 4.8             | 1117(3)                     | 1123(4)               | 1107(3)               | 1101(2) |
| 100        | 473      | 1.0             | 886(3)                      | 906(3)                | 906(3)                | 875(2)  |
|            |          | 2.0             | 933(3)                      | –                     | –                     | –       |
|            |          | 3.0             | 968(2)                      | 981(3)                | 972(3)                | 945(2)  |
|            |          | 4.0             | –                           | 1013(4)               | 1000(2)               | 972(3)  |
|            |          | 4.8             | 1023(4)                     | 1034(4)               | 1016(2)               | 991(3)  |
| 1000       | 298      | 1.0             | 1079(2)                     | 1091(1)               | 1087(1)               | 1079(3) |
|            |          | 2.0             | 1101(2)                     | 1126(1)               | 1117(1)               | 1107(4) |
|            |          | 3.0             | 1141(2)                     | 1157(1)               | 1145(1)               | 1144(3) |
|            |          | 4.0             | 1167(3)                     | 1186(1)               | 1170(1)               | 1172(3) |
| 1000       | 373      | 1.0             | 1032(2)                     | 1043(2)               | 1041(2)               | 1018(1) |
|            |          | 2.0             | 1066(2)                     | –                     | –                     | –       |
|            |          | 3.0             | 1101(3)                     | 1106(3)               | 1096(2)               | 1083(2) |
|            |          | 4.0             | –                           | 1135(4)               | 1121(2)               | 1111(3) |
|            |          | 4.8             | 1149(2)                     | 1154(4)               | 1135(2)               | 1130(3) |
| 1000       | 473      | 1.0             | 950(2)                      | 964(2)                | 962(2)                | 917(1)  |
|            |          | 2.0             | 986(2)                      | –                     | –                     | –       |
|            |          | 3.0             | 1021(3)                     | 1031(2)               | 1021(2)               | 988(2)  |
|            |          | 4.0             | –                           | 1015(3)               | 1044(2)               | 1015(3) |
|            |          | 4.8             | 1068(3)                     | 1037(3)               | 1062(2)               | 1037(3) |

Table 5: Simulation results for the viscosity,  $\eta$ , of different model combinations. Statistical uncertainties are given as in Table 1.

| T<br>(K) | P<br>(bar) | $m$<br>(mol/kg) | $\eta$ (cP) |          |                       |                       |          |
|----------|------------|-----------------|-------------|----------|-----------------------|-----------------------|----------|
|          |            |                 | SPC/E+JC    | SPC/E+SD | Semiflex.<br>SPC/E+JC | Semiflex.<br>SPC/E+SD | Exp6+TF  |
| 373      | 2          | 0.0             | 0.248(5)    | 0.248(5) | 0.298(9)              | 0.298(9)              | 0.177(3) |
|          |            | 0.44            | 0.300(3)    | 0.302(4) | 0.330(9)              | 0.319(4)              | 0.198(3) |
|          |            | 1.0             | 0.323(3)    | 0.332(4) | 0.359(4)              | 0.362(5)              | 0.229(2) |
|          |            | 2.0             | 0.410(1)    | 0.384(7) | 0.445(7)              | 0.426(5)              | 0.260(4) |
|          |            | 3.0             | 0.474(8)    | 0.449(6) | 0.549(9)              | 0.483(7)              | 0.302(8) |
|          |            | 4.0             | 0.560(9)    | 0.512(6) | 0.644(8)              | 0.606(2)              | 0.360(9) |
| 473      | 20         | 0.0             | 0.135(2)    | 0.135(2) | 0.148(2)              | 0.148(2)              | 0.111(1) |
|          |            | 0.44            | 0.148(3)    | 0.146(1) | 0.159(2)              | 0.159(3)              | 0.124(1) |
|          |            | 1.0             | 0.167(4)    | 0.163(1) | 0.172(1)              | 0.180(9)              | 0.129(2) |
|          |            | 2.0             | 0.197(1)    | 0.191(4) | 0.215(5)              | 0.209(4)              | 0.148(1) |
|          |            | 3.0             | 0.234(2)    | 0.228(3) | 0.245(3)              | 0.238(4)              | 0.178(2) |
|          |            | 4.0             | 0.273(2)    | 0.261(2) | 0.292(5)              | 0.281(6)              | 0.203(4) |

Table 6: Simulation results for the vapor-liquid interfacial tension,  $\gamma$ , of different model combinations. Statistical uncertainties are given as in Table 1.

| T<br>(K) | $m$<br>(mol/kg) | $\gamma$ (mN/m) |          |                       |                       |
|----------|-----------------|-----------------|----------|-----------------------|-----------------------|
|          |                 | SPC/E+JC        | SPC/E+SD | Semiflex.<br>SPC/E+JC | Semiflex.<br>SPC/E+SD |
| 298      | 1.0             | 64(1)           | 64(1)    | 69(1)                 | 67(1)                 |
|          | 2.0             | 68(1)           | 68(1)    | 69(1)                 | 70(1)                 |
|          | 3.0             | 70(1)           | 69(1)    | 72(1)                 | 72(1)                 |
|          | 4.0             | 74(1)           | 73(1)    | 76(1)                 | 76(1)                 |
| 373      | 1.0             | 52(1)           | 53(1)    | 56(1)                 | 57(1)                 |
|          | 2.0             | 56(1)           | 55(1)    | 59(2)                 | 58(1)                 |
|          | 3.0             | 57(1)           | 59(1)    | 60(1)                 | 62(1)                 |
|          | 4.0             | 62(2)           | 60(1)    | 64(1)                 | 63(1)                 |
| 473      | 1.0             | 33(1)           | 33(1)    | 36(3)                 | 39(2)                 |
|          | 2.0             | 35(1)           | 34(1)    | 41(2)                 | 40(2)                 |
|          | 3.0             | 39(2)           | 40(2)    | 41(1)                 | 42(1)                 |
|          | 4.0             | 43(1)           | 42(2)    | 45(1)                 | 45(1)                 |

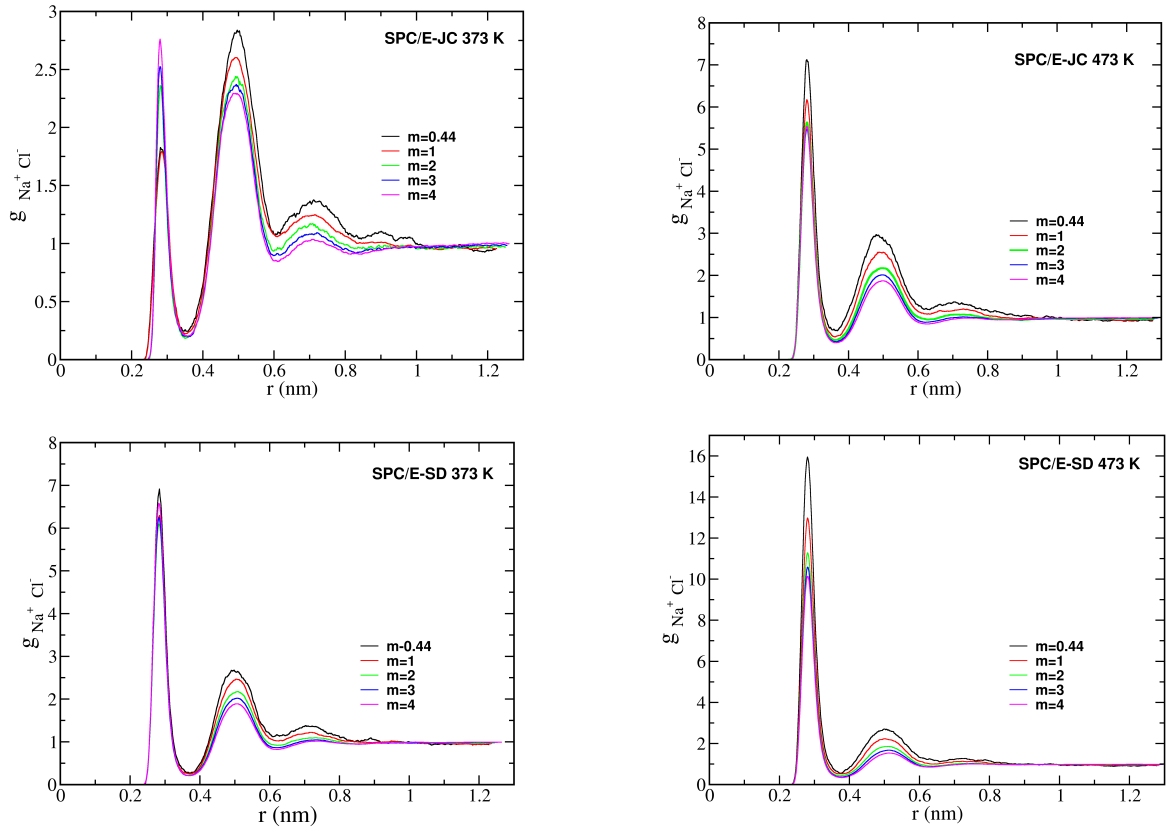


Figure 1: Pair correlation functions for the SPC/E model combinations.

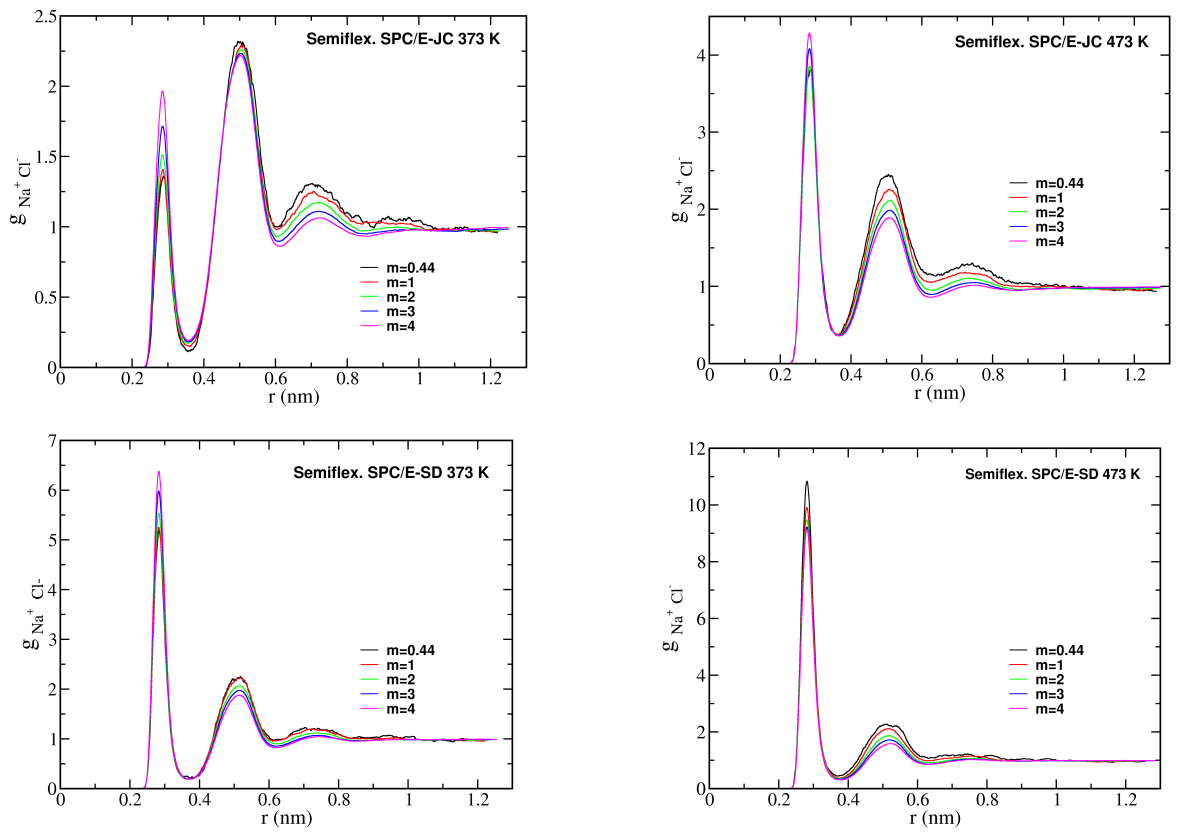


Figure 2: Pair correlation functions for the semiflexible SPC/E model combinations.

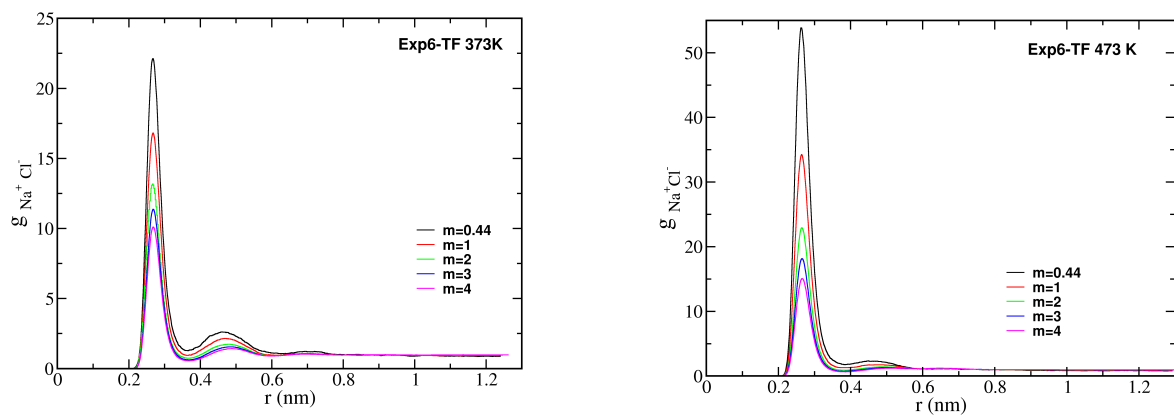


Figure 3: Pair correlation functions for the exp6+TF model combination.