Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supporting Information for: Developing Semi-Empirical Water Model for Efficiently Simulating Temperature-Dependent Chemisorption of CO_2 in Amine Solvents

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......
      METHOD  XTB
      &XTB
        DO_EWALD  T
        DO_NONBONDED  T
        CHECK_ATOMIC_CHARGES  F
        &PARAMETER
          DISPERSION_PARAMETER_FILE dftd3.dat
        &END PARAMETER
        &NONBONDED
          DX     1.0000000000000000E-03
          ERROR_LIMIT     1.0000000000000000E-10
          &GENPOT
            ATOMS O O
            FUNCTION epsilon*(-cos((r-sigma)*3.1415926/b)+0.45)/(1.0+exp((r-b1)/b2))
            VARIABLES r
            PARAMETERS epsilon sigma b b1 b2
            VALUES     7.1999999999999994E-04    8.6957000000000004E+00    3.0246000000000000E+00    8.8847000000000005E+00 \
                5.6710000000000005E-01
            RCUT     6.2000000000000002E+00
            RMIN     3.0000000000000013E+00
            RMAX     6.2000000000000064E+00
          &END GENPOT
        &END NONBONDED
      &END XTB
......
```

Figure S1: An example of the input script (for the cp2K 8.2 version) for the modified xTB method.

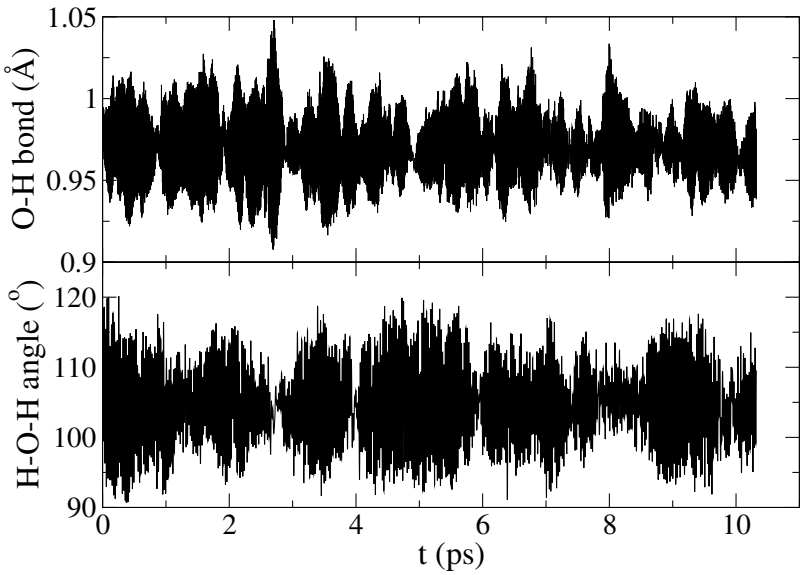

Figure S2: Time-dependent O-H bond lengths and H-O-H angles from the MD simulation for a box of water at 1 bar and 300 K, using the xTB-M model. The mean bond length is 0.97 Å with a root-mean-square-deviation (RMSD) of 0.02 Å, and the mean angle is 104.8° with a RMSD of 5.8°.

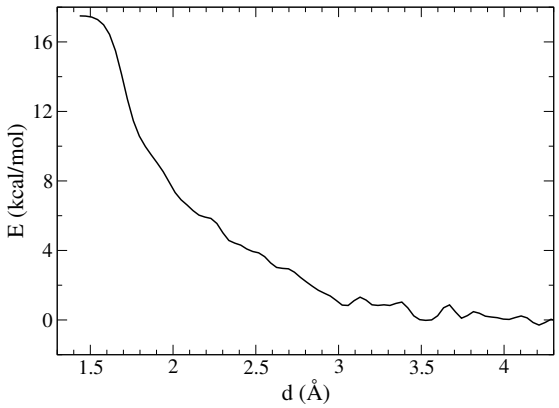

Figure S3: Free energy landscape for the zwitterion formation between MEA and CO2 in the gas phase at 300 K.

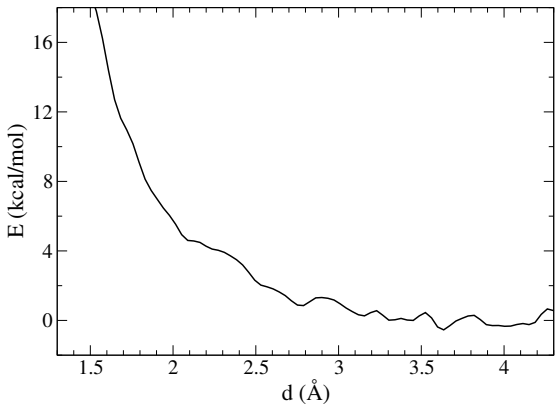

Figure S4: Free energy landscape for the zwitterion formation between MEA and CO2 in the implicit water (the SCCS method) at 300 K.

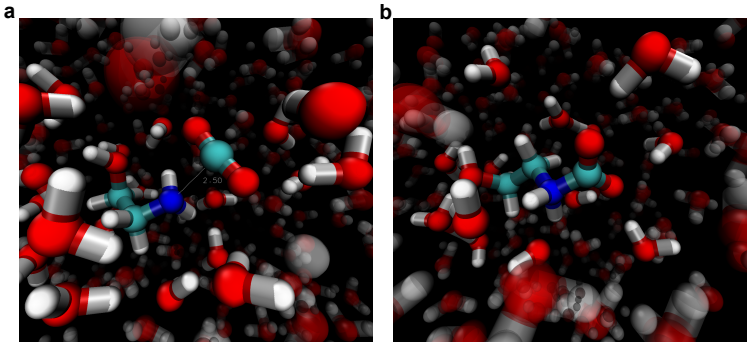

Figure S5: Representative states of the MEA-CO_2 complex in a water cage. a) The transition state (TS), where the N-C distance is 2.50 Å. ; b) The Zwitterion state, where the N-C bond length is about 1.65 Å.

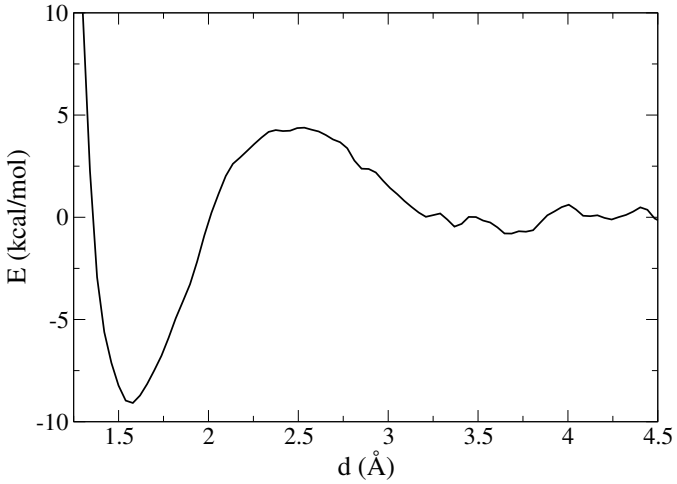

Figure S6: Free energy landscape for the zwitterion formation between MEA and CO2 at 300 K, with the explicit water using the unmodified xTB method.

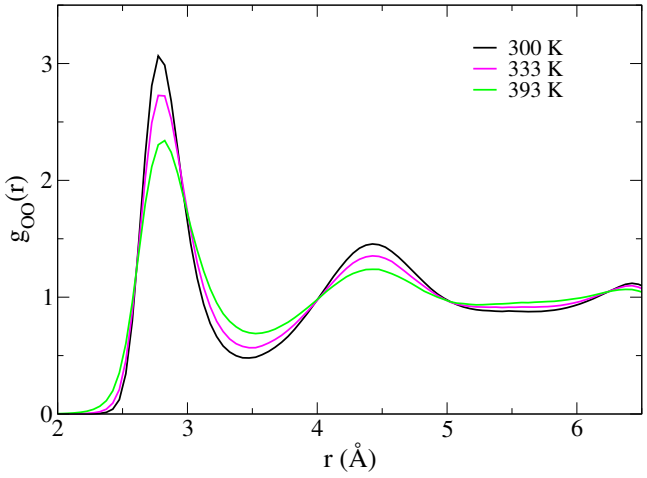

Figure S7: Radial distribution functions (RDF) for O-O pairs in water calculated from the xTB-M method, when T=300, 333 and 393 K.