Multi-factor study of the effects of a trace amount of water vapor on the low concentration CO$_2$ capture by 5A zeolite particle

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Table S1 L–J and particle charges of 5A zeolite and CO$_2$, N$_2$ and water molecule

(a) L–J parameters of 5A zeolite and CO$_2$, N$_2$ and water molecule

| Atom         | Atom         | $\sigma$ (Å) | $\varepsilon$ / $k_B$ (K) |
|--------------|--------------|--------------|--------------------------|
| O$_{\text{zeolite}}$ | C$_{\text{CO}_2}$ | 3.193 | 29.116 |
| O$_{\text{zeolite}}$ | O$_{\text{CO}_2}$ | 3.067 | 23.433 |
| Na           | C$_{\text{CO}_2}$ | 2.827 | 66.778 |
| Na           | O$_{\text{CO}_2}$ | 2.707 | 54.762 |
| Ca           | C$_{\text{CO}_2}$ | 2.944 | 96.932 |
| Ca           | O$_{\text{CO}_2}$ | 2.833 | 77.152 |
| Al           | C$_{\text{CO}_2}$ | 3.366 | 32.215 |
| Al           | O$_{\text{CO}_2}$ | 3.246 | 25.323 |
| Si           | C$_{\text{CO}_2}$ | 3.620 | 49.754 |
| Si           | O$_{\text{CO}_2}$ | 3.494 | 38.900 |
| C$_{\text{CO}_2}$ | C$_{\text{CO}_2}$ | 2.757 | 28.129 |
| O$_{\text{CO}_2}$ | O$_{\text{CO}_2}$ | 3.033 | 80.507 |
| O$_{\text{CO}_2}$ | C$_{\text{CO}_2}$ | 2.895 | 47.588 |
| O$_{\text{zeolite}}$ | O$_{\text{TIP4P}}$ | 3.421 | 51.734 |
| Al           | O$_{\text{TIP4P}}$ | 3.613 | 56.948 |
| Si           | O$_{\text{TIP4P}}$ | 3.887 | 87.850 |
| Ca           | O$_{\text{TIP4P}}$ | 3.157 | 171.814 |
| Na           | O$_{\text{TIP4P}}$ | 3.024 | 119.146 |
| O$_{\text{zeolite}}$ | H$_{\text{TIP4P}}$ | 0 | 0 |
| Al           | H$_{\text{TIP4P}}$ | 0 | 0 |
| Si           | H$_{\text{TIP4P}}$ | 0 | 0 |
| Ca           | H$_{\text{TIP4P}}$ | 0 | 0 |
| Na           | H$_{\text{TIP4P}}$ | 0 | 0 |
| O$_{\text{zeolite}}$ | L$_{\text{TIP4P}}$ | 0 | 0 |
| Al           | L$_{\text{TIP4P}}$ | 0 | 0 |
| Si           | L$_{\text{TIP4P}}$ | 0 | 0 |
| Ca           | L$_{\text{TIP4P}}$ | 0 | 0 |
| Na           | L$_{\text{TIP4P}}$ | 0 | 0 |
| O$_{\text{TIP4P}}$ | O$_{\text{TIP4P}}$ | 3.154 | 78.021 |
| L$_{\text{TIP4P}}$ | O$_{\text{TIP4P}}$ | 0 | 0 |
### Particle charges of 5A zeolite structure and CO$_2$ molecule

| Atom    | Si    | Na     | Al    | O_zeolite | Ca     | C_CO2  | O_CO2  |
|---------|-------|--------|-------|-----------|--------|--------|--------|
| Charge(e) | 2.2124 | 0.9887 | 2.0833 | -1.298    | 1.7166 | 0.6512 | -0.3256 |

| Atom    | O_TIP4P | H_TIP4P | L_TIP4P | N_N2     | N_com  |
|---------|---------|---------|---------|----------|--------|
| Charge(e) | 0       | 0.52    | -1.04   | -0.4048  | 0.8096 |
Table S2 Simulation parameters

| Property | Formula | values |
|----------|---------|--------|
| $Z$      | $Z^3 - \left(1 - \frac{bp}{RT}\right)Z^2 + \left(\frac{ap}{R^2T^2} - 3\frac{b^2p^2}{RT^2} - 2\frac{bp}{RT}\right)Z - \left(\frac{abp^3}{R^2T^2} - \frac{b^2p^2}{R^2T^2} - \frac{b^3p^3}{RT^2}\right) = 0$ | – |
| $a$      | $a = 0.45724 \frac{RT^2}{p_c} \left[1 + (0.37464 + 1.54226\omega - 0.26992\omega^3)(1 - T_c^{0.5})\right]^2$ | – |
| $b$      | $b = 0.07779 \frac{RT}{p_c}$ | – |
| $\Lambda$ | $\Lambda = \sqrt{\frac{h^2}{2\pi mkT}}$ | $h = 6.626 \times 10^{-34}$ Js |
|          |                                                   | $m_{co2} = 7.307 \times 10^{-26}$ kg |
|          |                                                   | $m_{N_2} = 3.32 \times 10^{-27}$ kg |

References

(1) D.Y. Peng and D. B. Robinson, A new two-constant equation of state, Ind. Eng. Chem. Fundam. 1976, 15, 59-64.