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Addition/Correction

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Corrections to "Understanding Adsorption and Transport of Light Gases in Hierarchical Materials Using Molecular Simulation and Effective Medium Theory"

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Recently we have become aware of two typographical errors and a minor numerical error in this article, which are reported below. None of these affects the results or conclusions of the article.

Correction 1

The formula for $(KD)_{mix}$ on page 14360 should be $(KD)_{mix} = [-a \pm (a^2 + 8b)^{1/2}]/4$; coefficients a and b are the same as in the publication: $a = (1-3\phi)K_{micro}D_{micro} - (2-3\phi)K_{meso}D_{meso}$ and $b = K_{micro}D_{micro}K_{meso}D_{meso}$. All the calculations were performed with the correct formula.

Correction 2

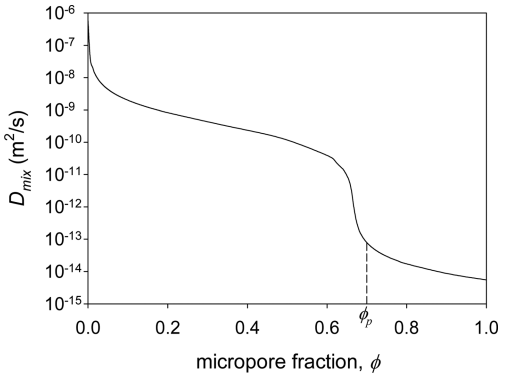
In page 14362, the collective diffusivity D_c of ethane in the flexible $AlPO_4$-34 structure is given as 1.0×10^{-10} m^2 s^{-1}. The correct value is 1.0×10^{-11} m^2 s^{-1}. This typographical error does not affect the analysis and conclusions from this work.

Correction 3

In eq 22, the diffusivity of propene in the mesopore space $D_{meso(prop)}$ is estimated from that of ethane $D_{meso(eth)}$ by simple rescaling

$$D_{meso(prop)} = D_{meso(eth)}\sqrt{\frac{M_{eth}}{M_{prop}}}$$

where M_{eth} and M_{prop} are the molar masses of ethane and propene, respectively. Fitting of the experimental uptake produces $D_{meso(eth)} = 7.0 \times 10^{-7}$ m^2 s^{-1}, which in turn yields $D_{meso(prop)} = 5.9 \times 10^{-7}$ m^2 s^{-1} as opposed to the value $D_{meso(prop)} = 1.3 \times 10^{-7}$ m^2 s^{-1}, incorrectly given. In this case Figure 12 is corrected as depicted below.



The qualitative shape of the curve remains the same, with only minor quantitative differences from the curve originally given. Moreover, since the percolation threshold ϕ_p is unchanged the conclusions derived from this calculation are unaffected.

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