In silico screening of carbon-capture materials

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1. Uncertainties in The Energy Cost of Capturing Carbon

To analyze the effect of these uncertainties on the overall parasitic energies, we selected a set of materials that spanned the range of parasitic energies. To simulate the propagation of possible errors on the thermodynamic input parameters in the parasitic energy, we changed each of these values by multiplying the actual value of a parameters by a factor, which was randomly selected from the interval [0.8, 1.2], i.e., a maximum possible error is plus or minus 20% on each of the thermodynamic variables. In this way, we generated, for each of the selected parasitic energies, 25 different sets of parameters. Figure SI 1 shows how these uncertainties propagate for a given value of the parasitic energy. We see that for high values of the parasitic energy, the results are much more sensitive. The reason is that small changes in the Henry coefficient have a large effect on the parasitic energy. In contrast, for low values of the parasitic energy the results are robust. This is consistent with the observation that we have for these materials a very broad optimum. Hence, some variations in the parameters have little influence, as at slightly different conditions a very similar optimal parasitic energy can be found. As we are mainly interested in materials with a low parasitic energy, this analysis shows that a 20% uncertainty in the main thermodynamic parameters should not have a significant influence on our estimates of the parasitic energy.
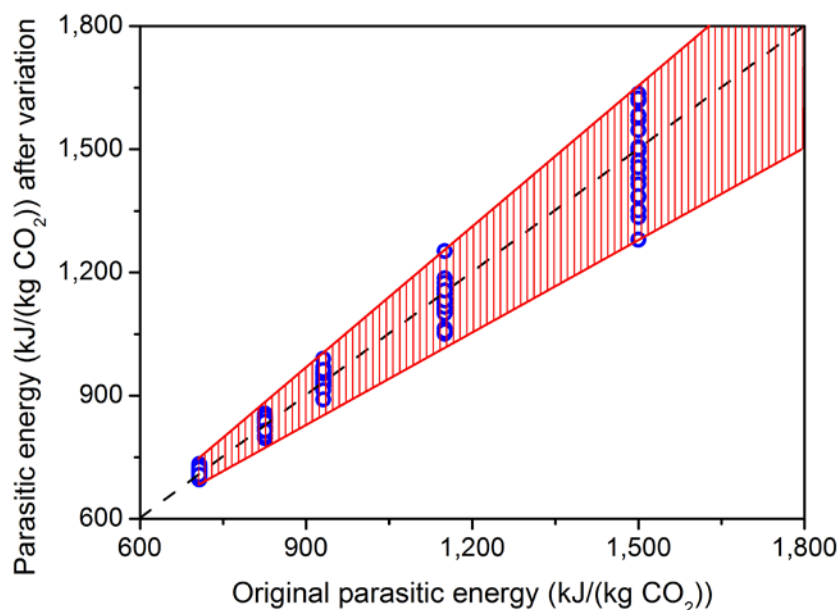
Figure SI 1: Uncertainties in the estimates of the parasitic energies. The blue dots are the 25 parameters sets for which we recalculated the parasitic energy after a change of +/- 20% of all parameters. The red line gives the upper and lower bounds of the errors in these sets.

2. Database of carbon capture materials

We have collected all results obtained in this work in a database, accessible at www.carboncapturematerials.org. The investigated materials have been characterized in terms of:

- Their pore geometry (pore measured by the diameter of the largest included and free spheres, accessible volume and surface areas),
- Adsorption properties (Henry coefficients and heats of adsorption for CO_2 and N_2, estimated Langmuir isotherms and in some cases simulated isotherms),
- Performance using the model discussed in the article (including parasitic energy, working capacity, and CO_2 purity).

The web interface allows the user to search for specific materials or materials with certain properties, and provides a graphical interface to browse the results. For example, plotting the parasitic energy as a function of the CO_2 Henry coefficient gives Figure 2a. In this figure each point is clickable and takes the user to the material entry page, which contains all the relevant properties for a particular material.

3. Detailed acknowledgements

4. Mixture Isotherms

The figures below show a comparison of the mixture isotherms as computed by molecular simulations (dots) with those predicted by the competitive isotherm model (lines) for a set of representative zeolite structures. The blue lines and symbols give the isotherms for N_2 and red lines and symbols the isotherms for CO_2.
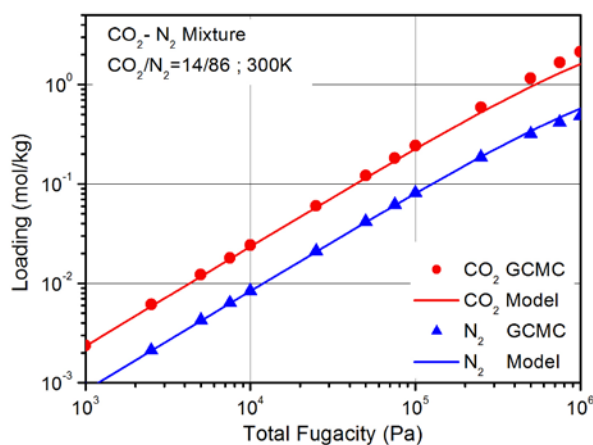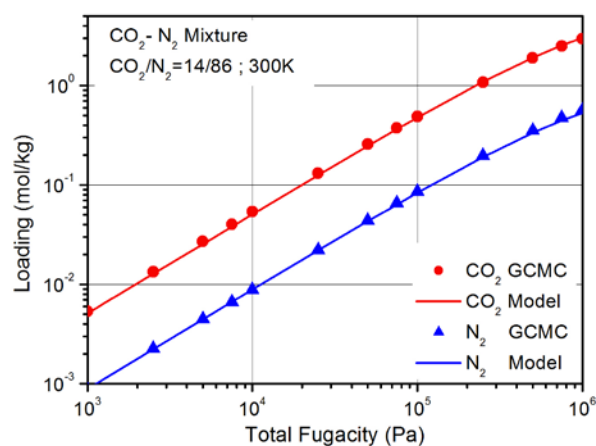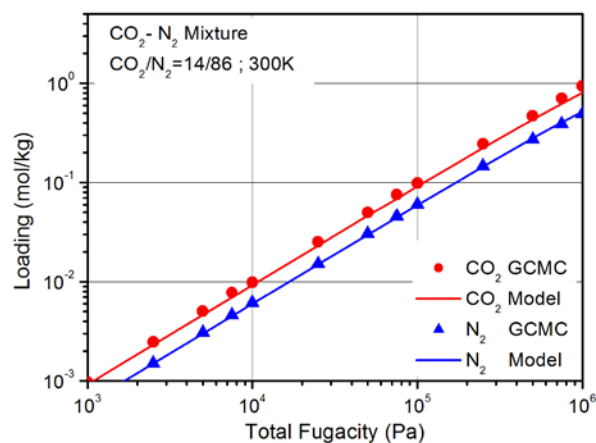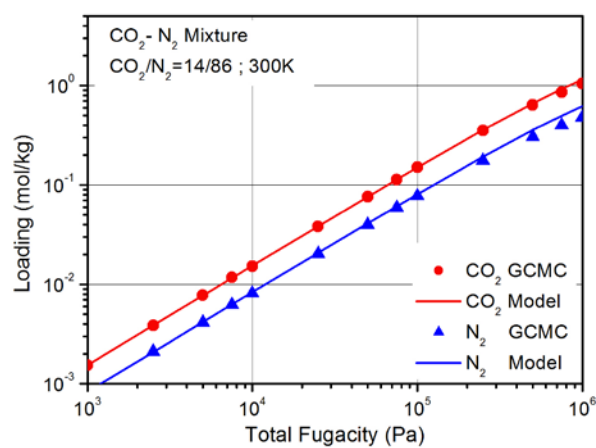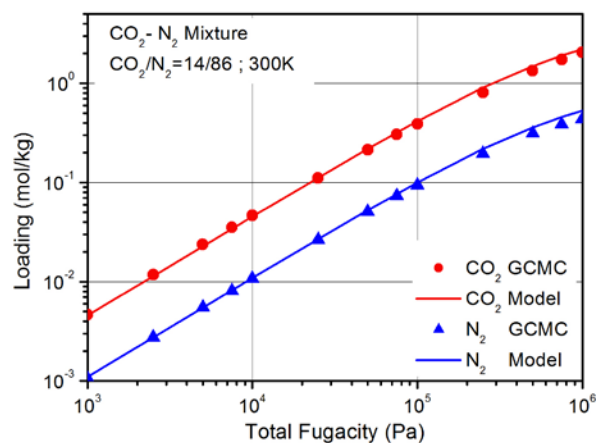

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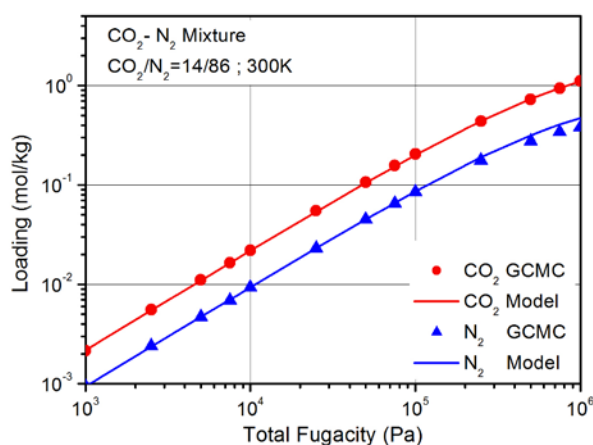
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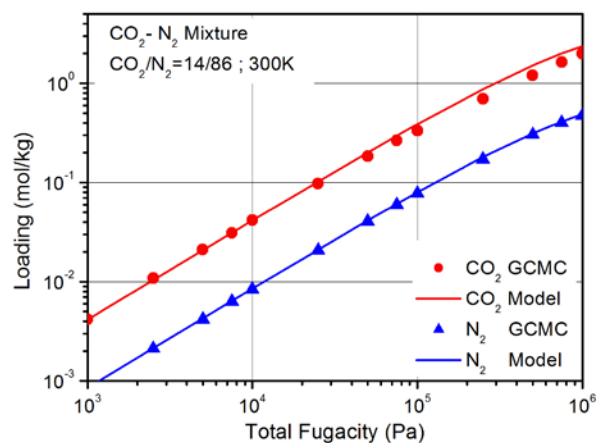
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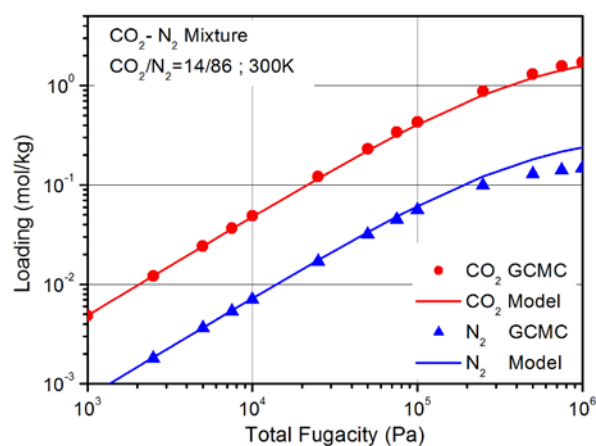
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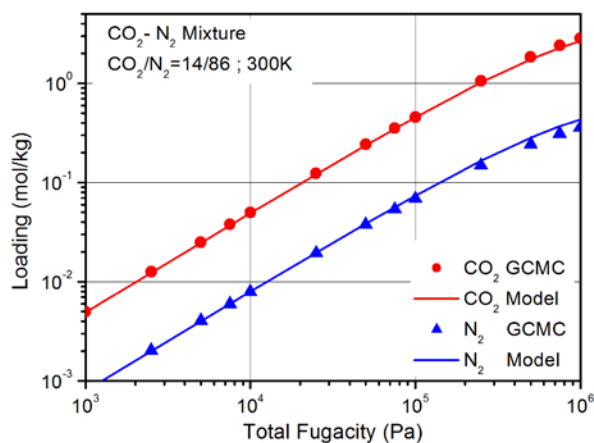
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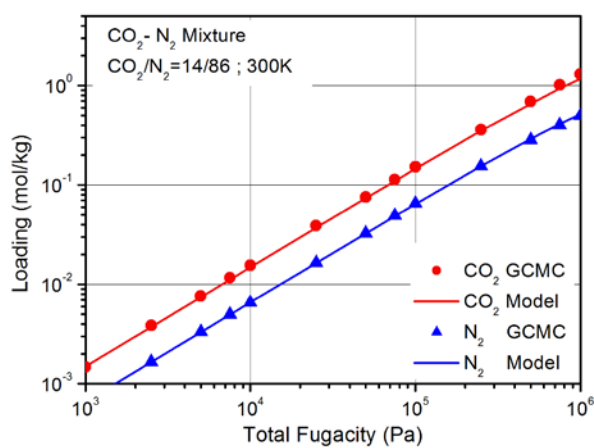
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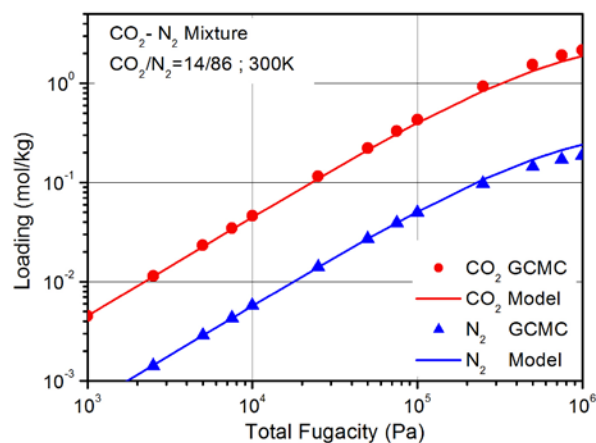
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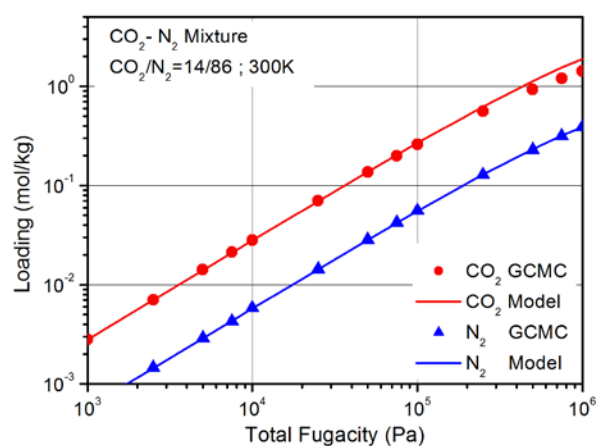
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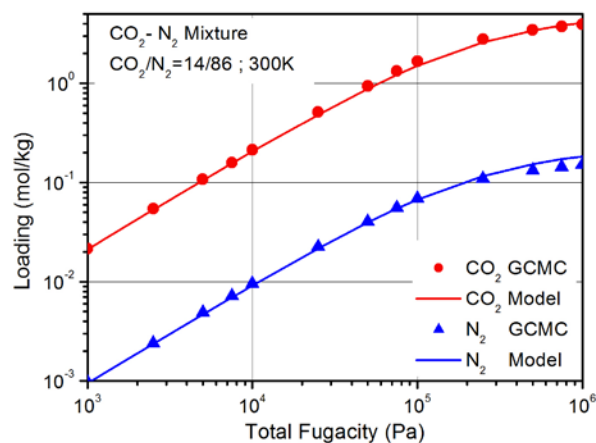
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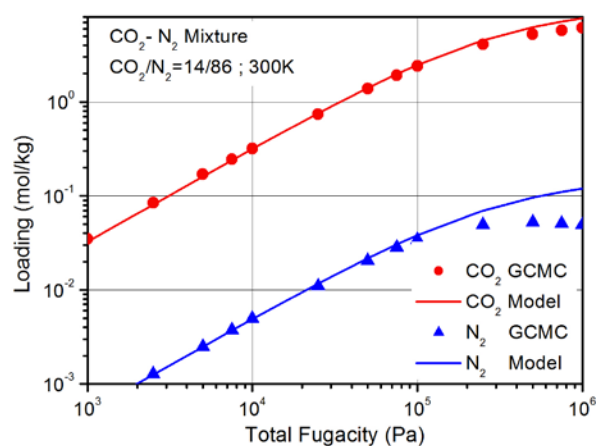
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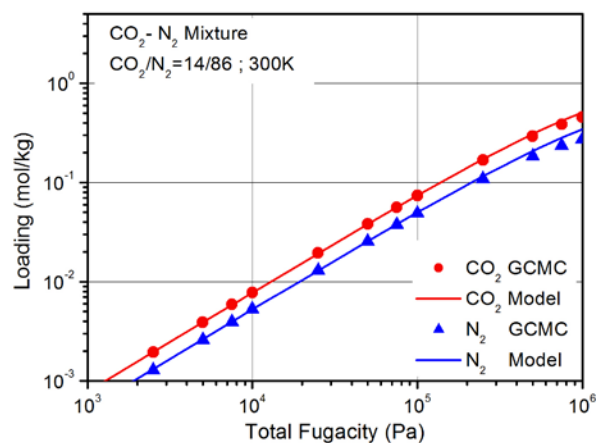
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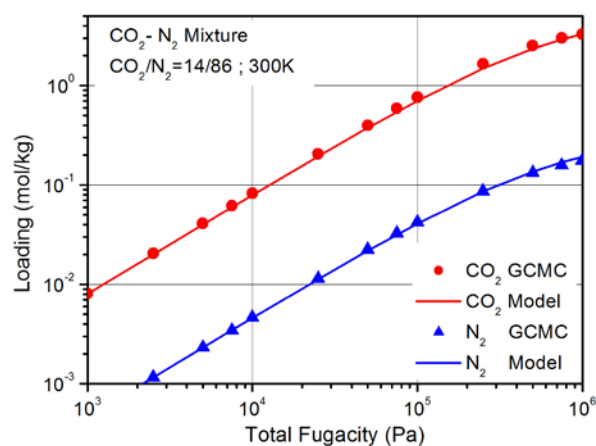
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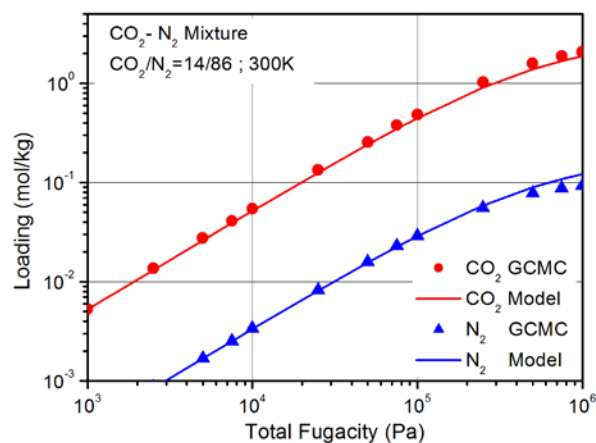
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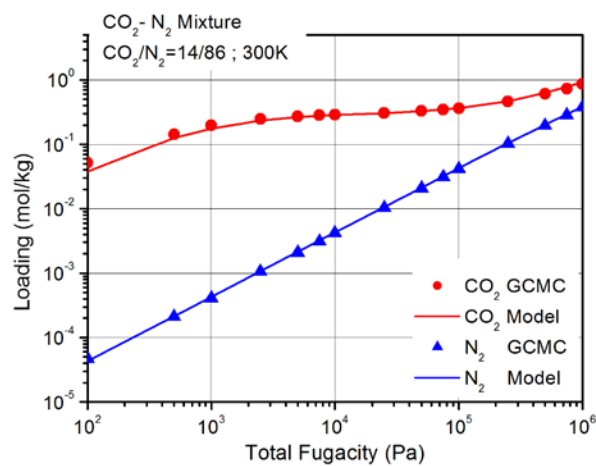
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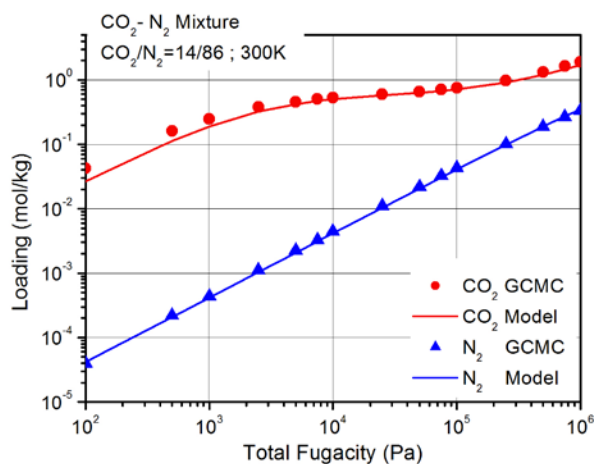
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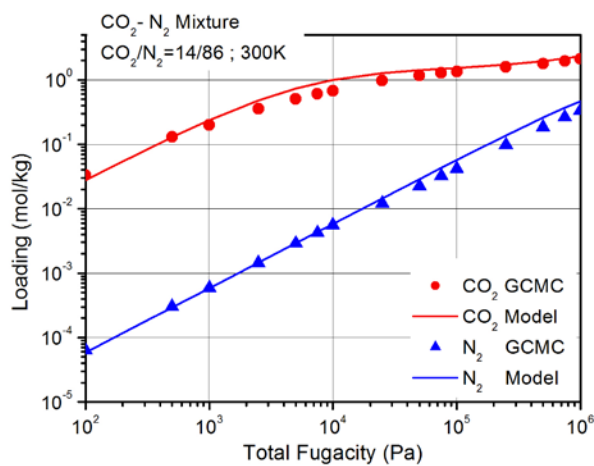
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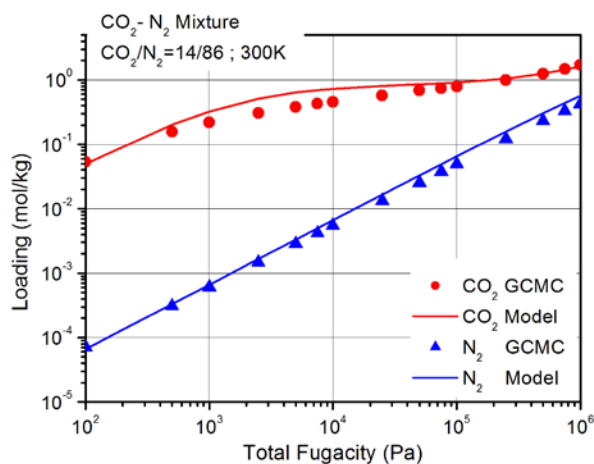
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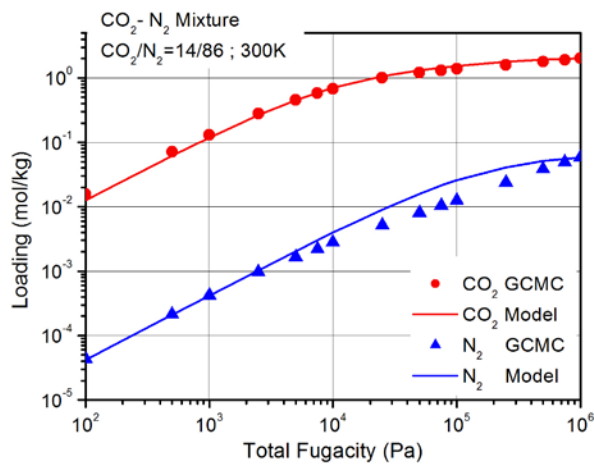
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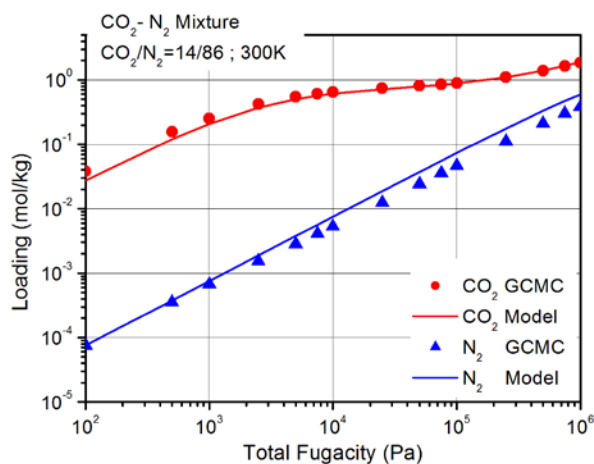
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