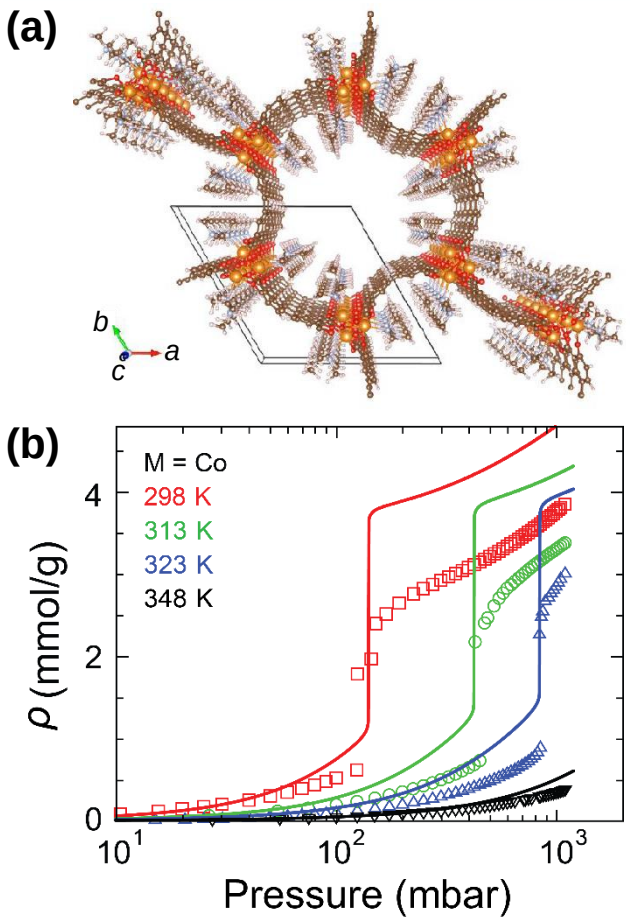
Cooperative Adsorption of Gas in a MOF Can Happen Even in the Absence of an Underlying Phase Transition



Cooperative adsorption of CO_2. (a) mmen-M_2(dobpdc). (b) Isotherms, at different temperatures (colors), from experiments (points) and simulations of our model (solid lines). The model reveals the mechanism underlying the sharp isotherm.

Scientific Achievement

A physical understanding of how the sharp CO_2 uptake isotherm in mmen–M_2(dobpdc) results from the polymerization of CO_2 chains, absent a phase transition

Significance and Impact

Knowing the underlying mechanism reveals how to change the properties of the isotherm for experimental and industrial convenience

Research Details

– A combination of quantum- and statistical mechanics was used to build a physical model of CO_2 uptake in mmen–M_2(dobpdc) (mmen = *N*,*N*′-dimethylethylene-diamine; dobpdc^{4-} = 4,4′-dioxido-3,3′-biphenyldi-carboxylate; M = Mg, Mn, Fe, Co, Zn, and Ni). Analysis of the model reveals the origin of the sharp isotherm.

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