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In situ CO_2 adsorption by the (poly)azolate MOF Fe_2BPEB_3

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Developing new adsorbents for CO2 capture and storage is critically important. In the past fifteen years, metal–organic frameworks (MOFs) (1) have emerged as promising materials for the selective adsorption of CO2 (2). In general, most research efforts in this area have focused on either increasing MOFs pore volume and surface area to increase CO2 adsorption capacity, or modifying pore chemistry by incorporating functional moieties having high affinity for CO2.
We have recently shown (3) that the rigid MOF Fe2(BPEB)3 [H2BPEB = 1,4-bis(1H-pyrazol-4-ylethynyl)benzene] adsorbs up to 40.5 wt % of CO2 under the rather mild conditions of 298 K and 10 bar, this occurrence placing it among the best performing MOFs under the same experimental conditions.
After in situ and operando high-resolution and high-energy powder X-ray diffraction experiments, by combining conventional structural analysis to pair distribution function analysis and molecular dynamics simulations, we provided a coherent picture of the preferential adsorption sites and host-guest and guest-guest interactions characterizing CO2 adsorption in Fe2(BPEB)3 at 298 K and in the pressure range of 0-20 bar. Our molecular-level insight into the nature of the host-guest interactions in Fe2(BPEB)3, a host without exposed metal sites or functional groups with particular affinity to CO2 on the ligand, not only sheds light on the Fe2(BPEB)3/CO2 system, but also provides key information on a debated topic, namely the chemical and structural properties a host should possess for efficient CO2 adsorption even under rather mild conditions.
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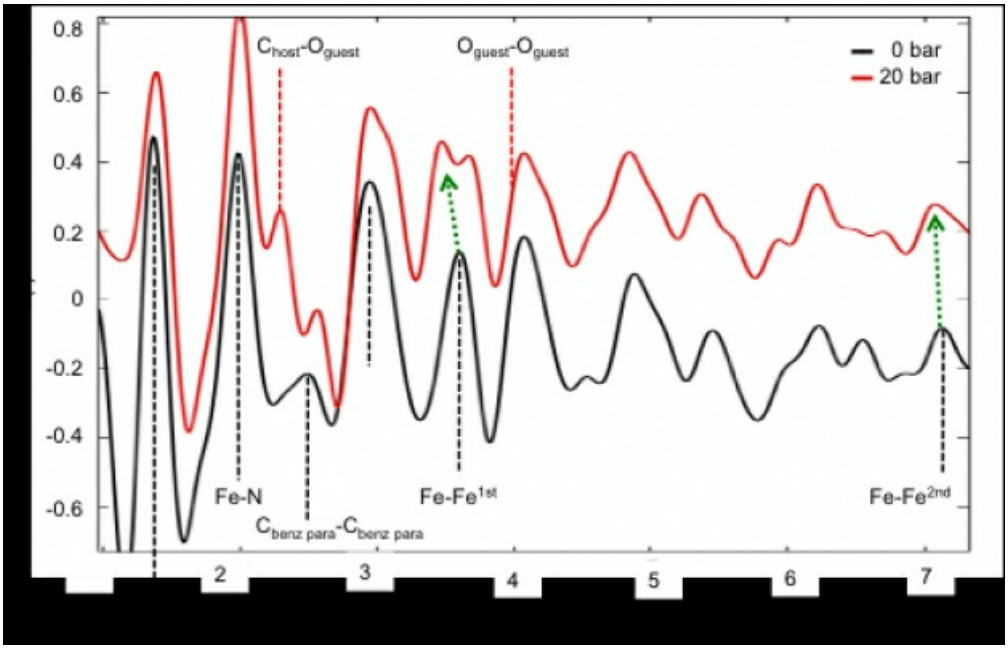

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