**Reversible CO Scavenging via Adsorbate-Dependent Spin Transitions in an Fe(II)–Triazolate Metal–Organic Framework**

**Scientific Achievement**
A metal–organic framework featuring Fe(II) sites that reversibly and selectively convert between high- and low-spin forms upon CO binding, via a novel spin transition mechanism.

**Significance and Impact**
This material exhibits high selectivity for trace amounts of CO over H₂, N₂, and even strongly binding gases like CO₂, making it useful for production of pure H₂ or extraction of waste CO from industrial feeds. The associated spin transition mechanism can also potentially be used for other selective separations.

**Research Details**
- Fe-BTTri adsorbs CO at low partial pressures (1.45 mmol/g at 100 μbar) with very good selectivity over other gases (CO/H₂ IAST selectivity values reaching 10 000)
- Fe-BTTri is fully regenerable with heating for as little as 5 min
- Spin transition mechanism is supported by X-ray diffraction, Mössbauer spectroscopy, and SQUID magnetometry

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**Overview of spin transition mechanism and gas adsorption**


Work was performed at UC Berkeley and the Advanced Light Source at Lawrence Berkeley National Laboratory.