

# Separation of O<sub>2</sub> from N<sub>2</sub> on Fe<sub>2</sub>(dobdc)

- Separating O<sub>2</sub> from N<sub>2</sub> is an important chemical process and is currently done using cryogenic distillation in industry.
- Fe<sub>2</sub>(dobdc) has been found to be a promising cost-effective and energy-efficient alternative for this separation.<sup>1</sup>
- Theoretical calculations performed on Fe<sub>2</sub>(dobdc) explain the stronger binding of O<sub>2</sub> than N<sub>2</sub> based on charge transfer, bond order, orbital energies, and vibrational frequencies.<sup>2</sup>

1. Bloch, Murray, Queen, Chavan, Maximoff, Bigi, Krishna, Peterson, Grandjean, Long, Smit, Bordiga, Brown, Long. *J. Am. Chem. Soc.* **2011**, *133*, 14814.
2. Verma, Maurice, Truhlar. *J. Phys. Chem. C* **2015**, *119*, 28499. DOI: 10.1021/acs.jpcc.5b10382

