

Implementation of Hard-Soft Chemistry for one-Pot Synthesis of Bimetallic MOFs Suitable for Xe/Kr Separation

Konstantinos G. Froudas*, Giasemi K. Angeli, Pantelis N. Trikalitis

*Department of Chemistry, University of Crete, Voutes, Heraklion 71003, Greece
chemp1161@edu.chemistry.uoc.gr*

Metal-Organic Frameworks (MOFs) constitute a unique class of multifunctional, open-framework solids with prospective applications pertaining to energy and environmental sustainability. [1] To their vast majority, MOFs consist of inorganic and organic molecular building units, whose embedded geometrical information allows their regulated assembly under the principles of reticular chemistry. [2] Nevertheless, the systematic generation of more intricate structures, composed of two or more different metal ions by the practice of the aforementioned designing approach encounters noticeable limitations, mostly due to deviations in reaction kinetics.

In the present work, we report the one-pot rational construction of a mixed-metal-organic framework (M²MOF) by the deliberate implementation of hard and soft acid and base (HSAB) theory. [3] In particular, a bifunctional ligand comprised of a hard carboxylate and a soft pyrazolate moiety was purposely selected, aiming at the preferential binding of the former to a hard Lewis acid (M⁴⁺) and the latter to a soft Lewis acid (M²⁺). The resultant 3D framework with the rare **scu** underlying topology features comfortably accessible, 1D polygonal channels, while the synergism emerging from the highly polar pore environment (arising from different functionalities) and distinct structural characteristics is responsible for its notable performance in Xe/Kr separation.

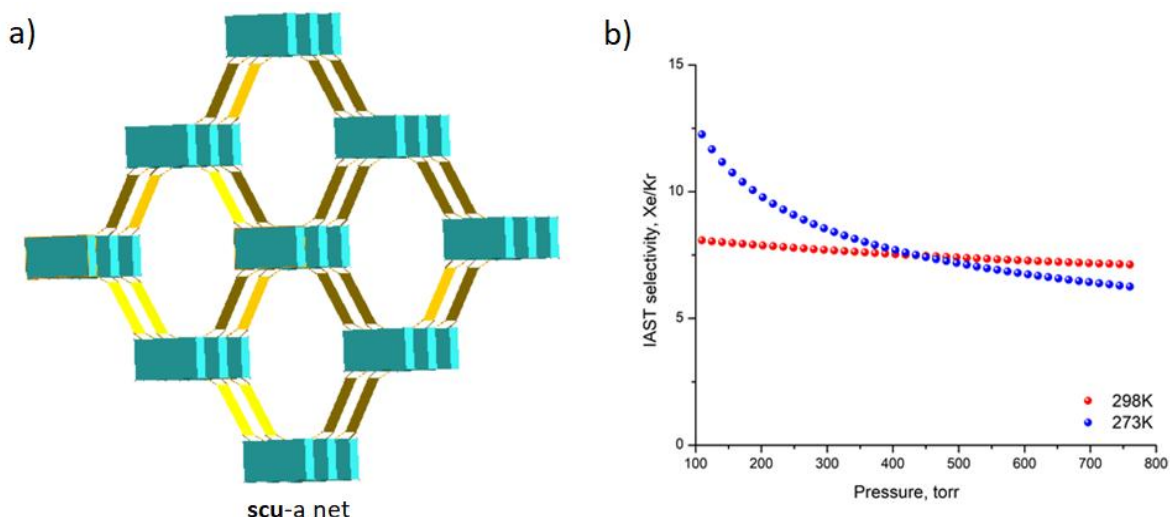


Figure 1: (a) The augmented **scu**-a net (b) Selectivity of Xe over Kr at 298 K and 273 K as predicted by IAST for a 10/90 Xe/Kr molar mixture.

References

- [1] Furukawa, K.E.; Cordova, K.E.; O’Keeffe, M. et al. *Science* **341**, 1230444 (2013).
- [2] Jiang, H.; Alezi, D.; Eddaoudi, M. *Nat. Rev. Mater.* **6**, 466-487 (2021).
- [3] Froudas, K.G.; Angeli, G.K.; Trikalitis, P.N. submitted (2022).