Molecular dynamics study of CO_2 absorption in zinc imidizolate frameworks

Min Gao,[†] Alston J. Misquitta,[†] Chengxing Yang,[†] Ilian T. Torodov,[‡]

Andreas Mutters,[¶] and Martin T. Dove[*,†]

[†]*School of Physics and Astronomy, and Materials Research Institute, Queen Mary University of London, Mile End Road, London, E1 4NS, UK*

[‡]*Scientific Computing Department, STFC Daresbury Laboratory, Sci-Tech Daresbury, Keckwick Lane, Daresbury, Cheshire, WA4 4AD, UK*

[¶]*Department of Earth Sciences, University of Cambridge, Downing Street, Cambridge, CB2 3EQ, UK; present address: Fachbereich Physik, Erwin-Schrödinger-Strasse, 67663 Kaiserslautern, Germany.*

E-mail: martin.dove@qmul.ac.uk

Abstract

This document contains supplementary data for the paper.

CO_2 density profile

Patterns of pore structure

Most of the ZIFs pores (ZIF-2,3,zni,10,6) have been occupied by CO_2 in figure 7. ZIF-8 is exceptional because our ZIF-8 has never reached the saturation state and only the first

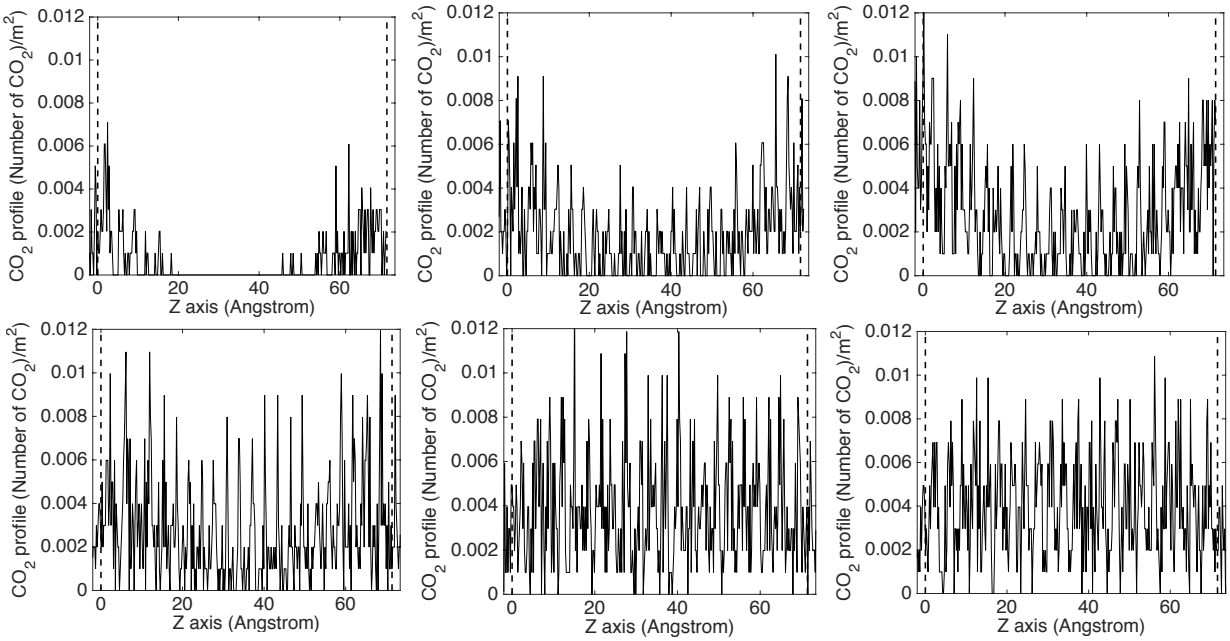


Figure 1: Absorbed CO_2 density profile at 81 ps, 408 ps, 858 ps,1527 ps, 5727 ps and 10665 ps in ZIF-zni. The Z axis is the axis normal to the slab.

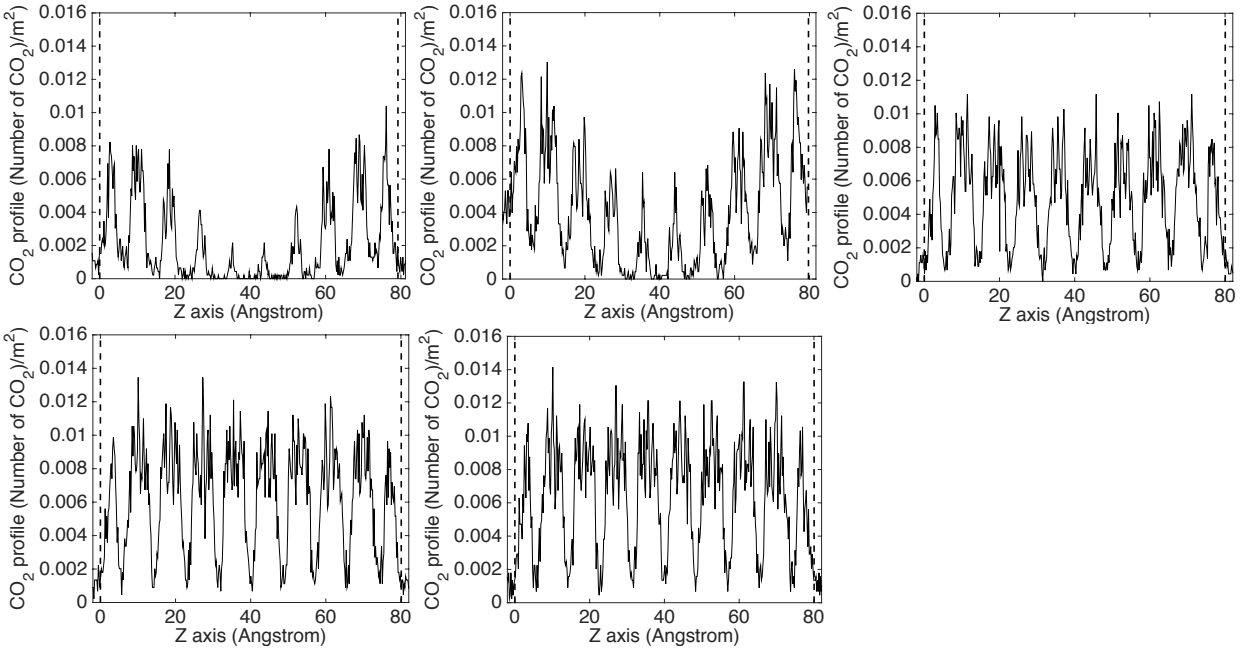


Figure 2: Absorbed CO_2 density profile at 213 ps, 366 ps, 840 ps, 2046 ps and 3318 ps in ZIF-3. The Z axis is the axis normal to the slab

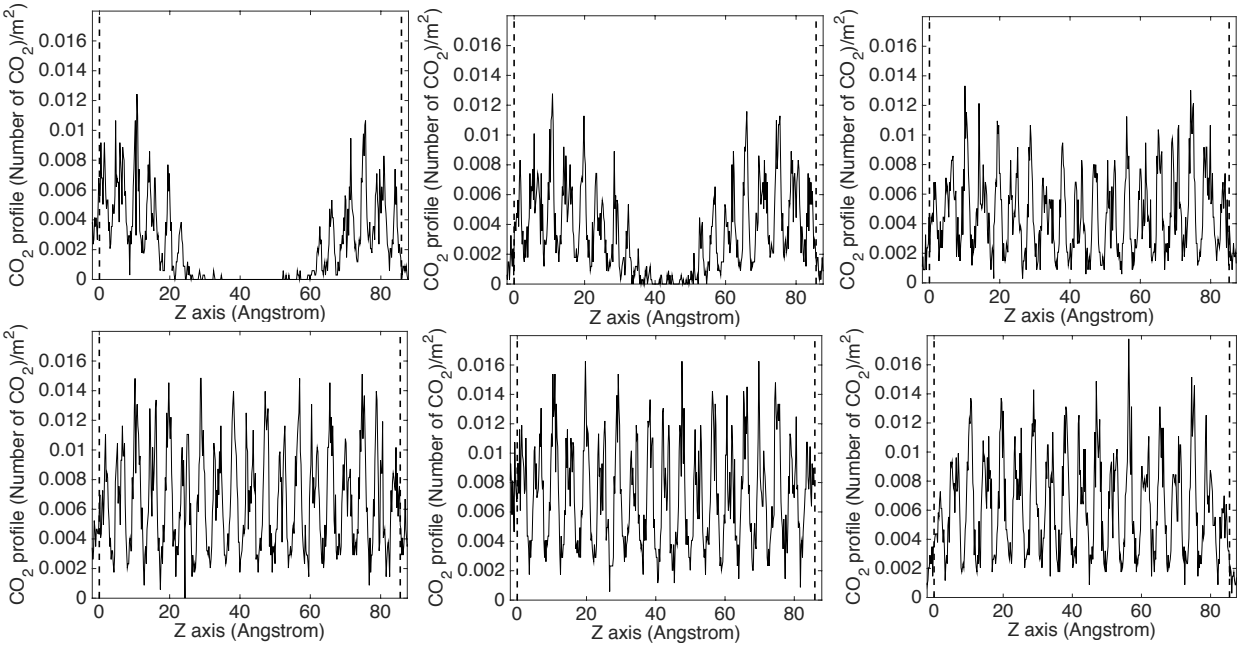


Figure 3: Absorbed CO_2 density profile at 381 ps, 798 ps, 1587 ps, 3432 ps, 3617 ps and 6084 ps in ZIF-4. The Z axis is the axis normal to the slab

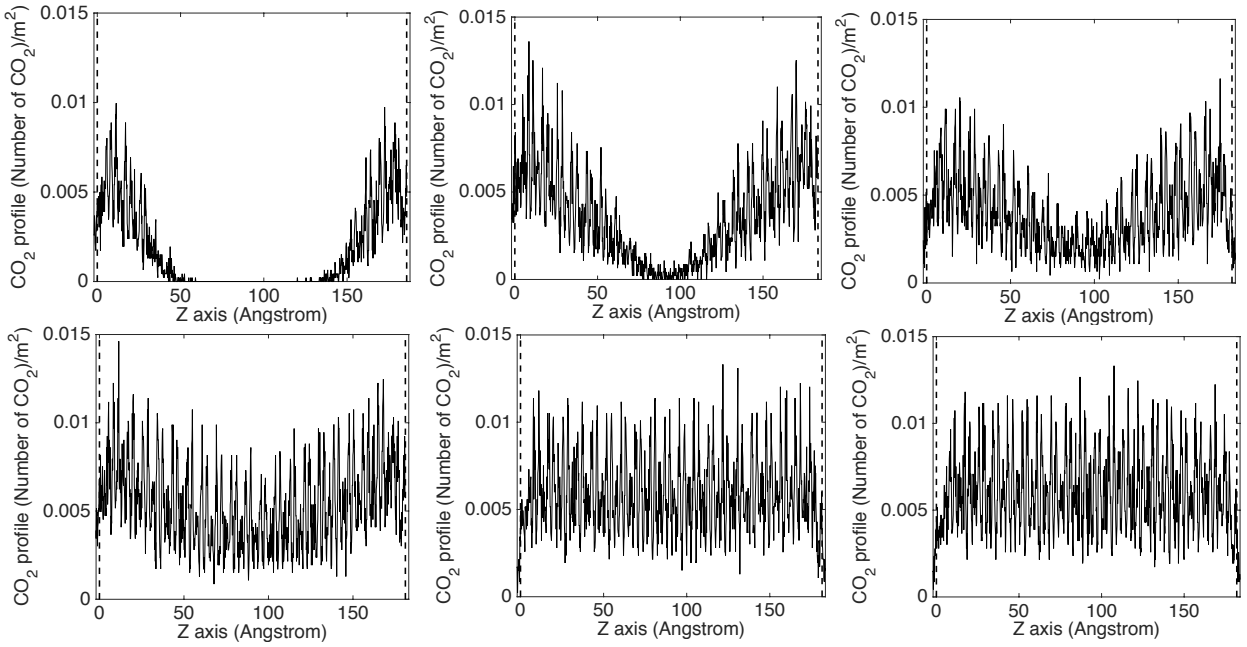


Figure 4: Absorbed CO_2 density profile at 405 ps, 1302 ps, 1908 ps, 2739 ps, 4734 ps and 12300 ps in ZIF-6. The Z axis is the axis normal to the slab

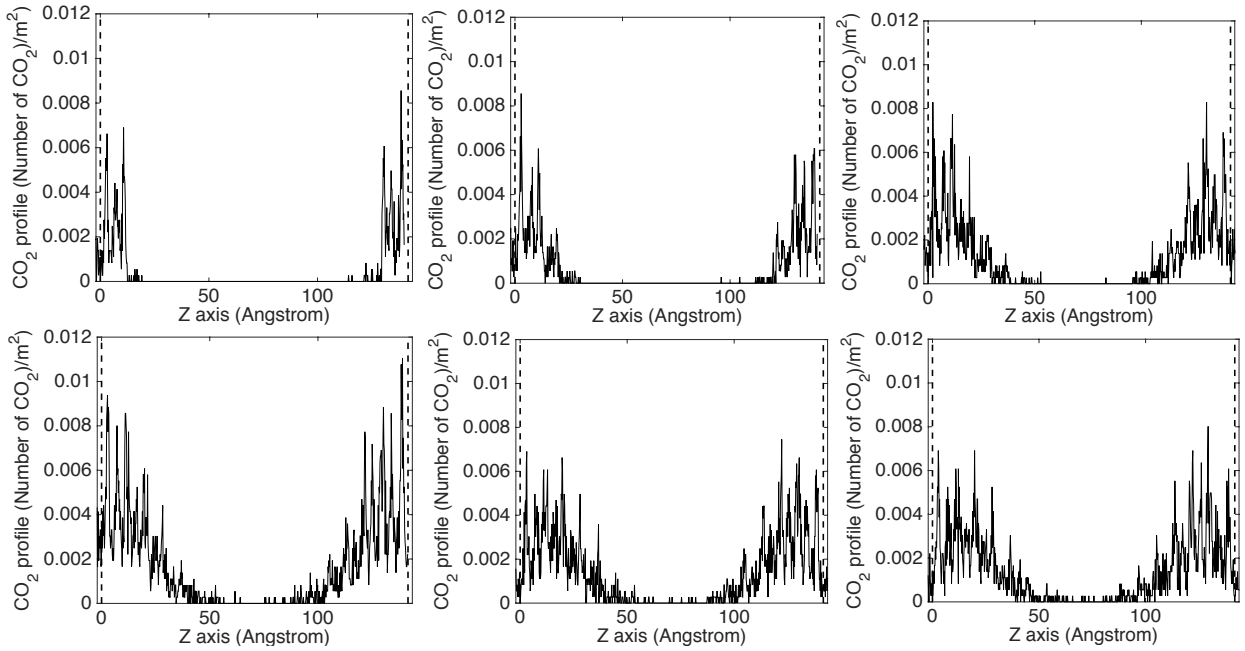


Figure 5: Absorbed CO_2 density profile at 300 ps, 3000 ps, 12711 ps, 20922 ps, 22734 ps and 25536 ps in ZIF-8. The Z axis is the axis normal to the slab

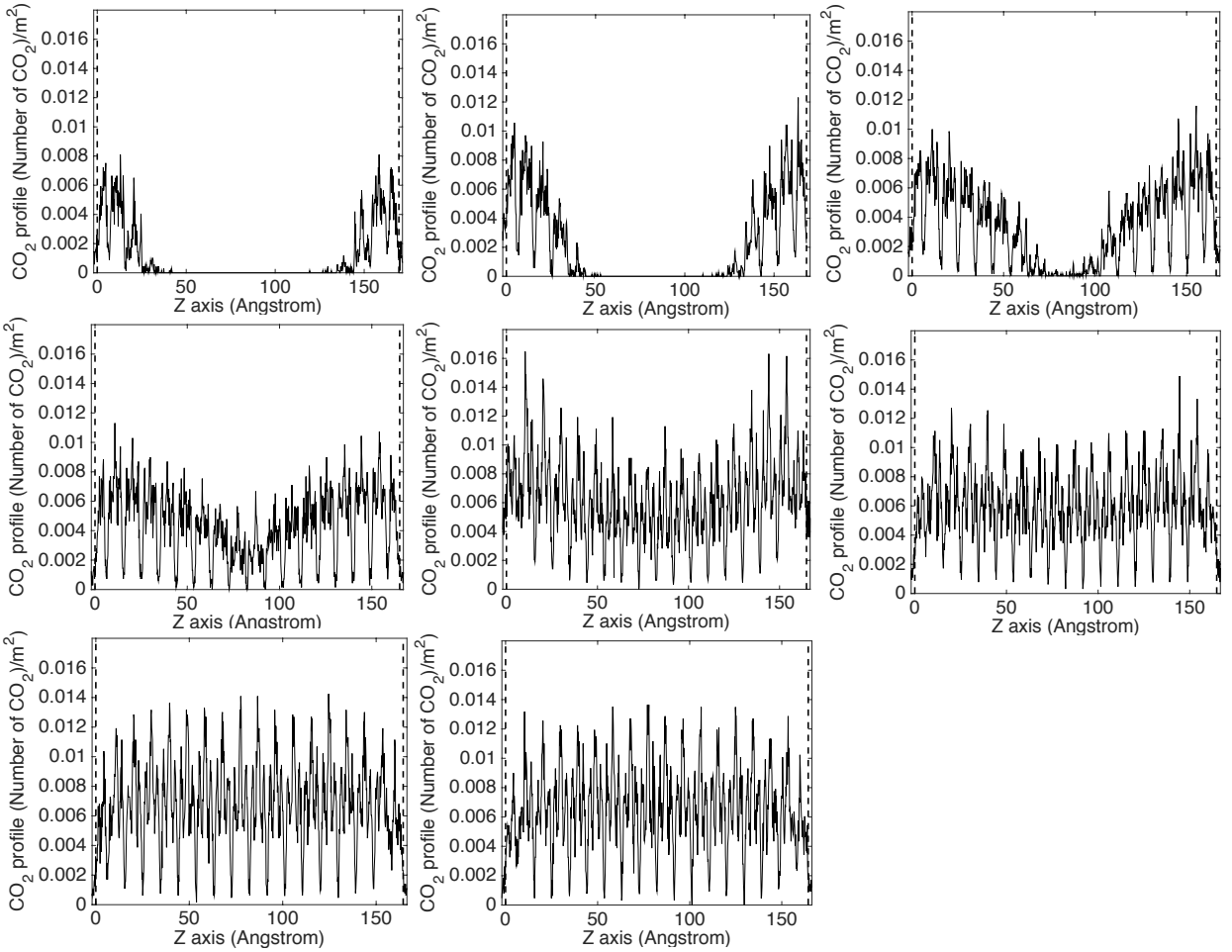
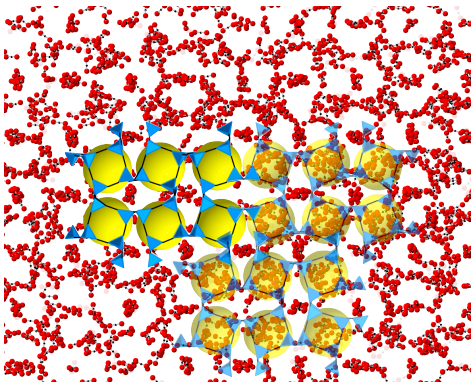
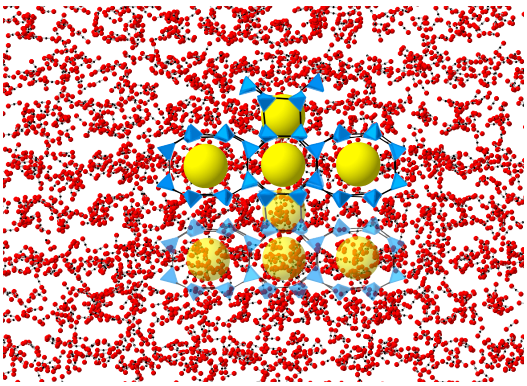


Figure 6: Density profile of absorbed CO_2 molecules and Zn atoms in saturated ZIF-10 at 200 °C, under 25 bar. The top three figures are from the beginning of the simulation (243 ps) and bottom three figures are the ones at saturation state.

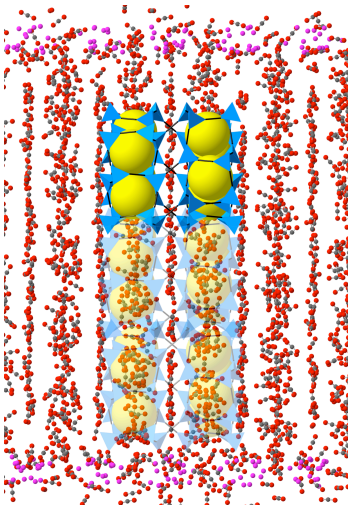
three layers has been occupied. However, it does show a trend that the CO_2 molecules been confined in the pores.



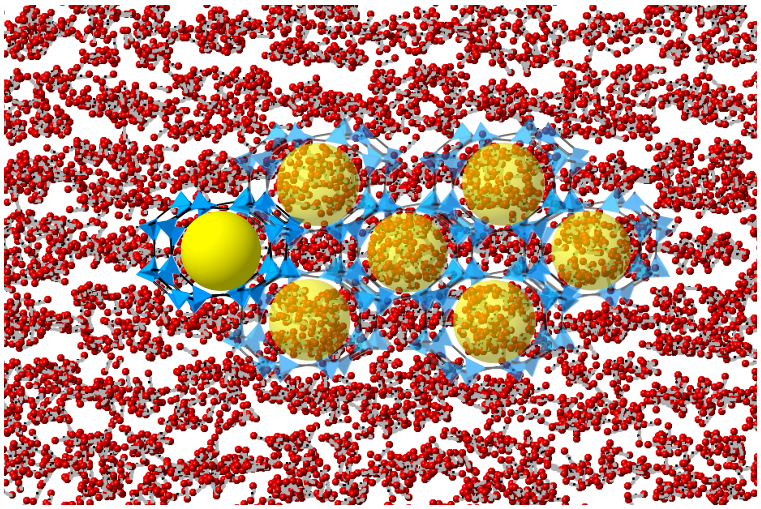
(a) ZIF-2



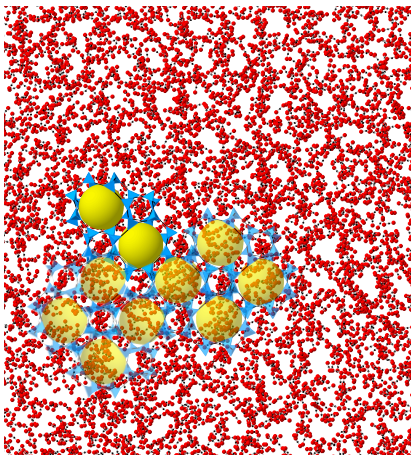
(b) ZIF-3



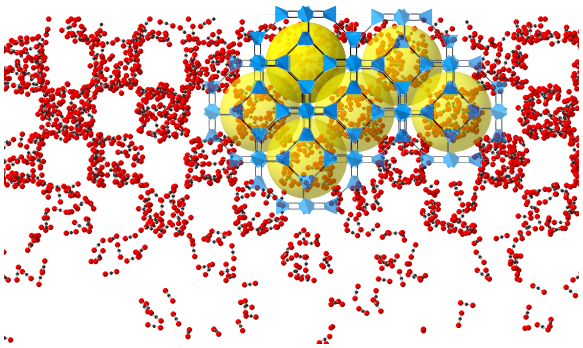
(c) ZIF-zni



(d) ZIF-10



(e) ZIF-6



(f) ZIF-8

Figure 7: CO_2 molecules inside ZIFs slabs at saturation sate without the ZIF atoms presented.