Supplementary Information

Computational details

Gulp programs[1] has been employed for the molecular dynamics simulations of C_{60} ion displacement in channels of Zn-MOF-74. The slab obtained from the supercell **1x1x4** of Zn-MOF-74 is used for simulations. The atoms of Zn-MOF-74 are frozen, apart of hydrogens and methyl groups. DREIDING force field[2] has been used to describe the interatomic interactions. Atomic charges have been obtained via QEq procedure[3]. Simulations have been performed at temperature 298K. Periodic boundary conditions are applied for the simulation cell. The time step during the simulation is 1 fs. Half of the atoms of nanotubes (6,6) are not frozen, another half is frozen. Atoms of nanotubes nearby to C_{60} are free. Duration of equilibration is 10 ps. Different starting position of C_{60} ion are used to make sure in reproducibility of results. Duration of production time is 14 ps.

Calculations of the memory element access rate

1 Thz = 10^{12} Hz

1 ps = 10^{-12} s

10 ps = 0.1 Thz

3.7 ps – time duration from bit 1 to bit 0

3.7 ps = 0.27027 Thz, please, see http://halas.rice.edu/conversions

0.1 Thz equal to 10 Gbyte/s

0.27027 Thz equal to 27.027 Gbyte/s

Unit conversion

Please, see
https://www.theunitconverter.com/megabit-second-to-megabyte-second-conversion/5000-megabit-second-to-megabyte-second.html

Calculations of memory density

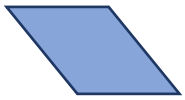
Units Conversion:

1 inch = 2.54e^{8} Å;

Converting 1 sqr inch to $Å^2$:

1 sqr inch = $6.452e^{16}$ $Å^2$;

Square of the unit cell - S:

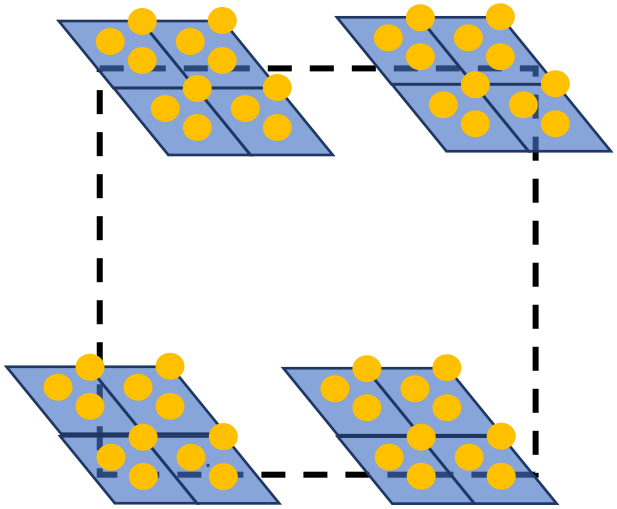


45.8395Å -length (a and b directions) of unit cell

S=45.8395Å x (45.8395 Å *cos30^o);

Cos30^o = 0.87

S=45.8395Å x 39.880365 Å=1828.096$Å^2$



The smaller the bit cells are, the better the storage density of the medium is.

$6.452e^{+16}$ $Å^2$/1828.096 $Å^2$= $3.53e^{13}$ unit cells per $inch^2$

$3.53e^{13}$*3 elements=$1.06e^{14}$ memory elements

Converting from bit to terabit

http://gowww.convert-units.info/data-storage/gigabyte/7.74E-13

106 Tb (terabit) per $inch^2$

Current achievement of *Seagate* is 2 Tb per $inch^2$:
https://blog.seagate.com/craftsman-ship/hamr-next-leap-forward-now/
Seagate prediction is to reach10 Tb per $inch^2$ in 2025

Notes and references

1. Gale, J. D. GULP: A computer program for the symmetry-adapted simulation of solids. *Journal of the Chemical Society, Faraday Transactions* **1997**, *93*, 629-637.

2. Mayo, S. L.; Olafson, B. D.; Goddard, W. A. DREIDING: a generic force field for molecular simulations. *The Journal of Physical Chemistry* **1990**, *94*, 8897-8909.

3. Rappe, A. K.; Goddard, W. A. Charge equilibration for molecular dynamics simulations. *The Journal of Physical Chemistry* **1991**, *95*, 3358-3363.