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Supplemental Information

Molecular simulation of low temperature argon adsorption in several models of IRMOF-1 with defects and structural disorder

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1. Forcefield parameters (Universal Force Field[1])

Atom type	σ, Å	ε, K
C	3.431	52.80
O	3.118	30.20
H	2.571	22.14
N	3.261	34.70
Zn	2.462	62.38
Ar	3.440	93.27
Au	2.934	19.61

2. Additional simulation details

Iterations, per adsorption point	$40 \cdot 10^6$ - $80 \cdot 10^6$
Cut-off (Å)	12.8 (no tail corrections)
Type of moves	Insertion, deletion, translation, rotation (for non-spherical species)
Weight of each type of move	Equal weight
Iterations used for equilibration	50%
Iterations used for statistical sampling	50%
α and shield parameters for the Fennell-Gezelter	0.1, 1.0

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method [2]	
K_{MAX} (number of unit cell images in the reciprocal space), κ (parameter related to the width of the Gaussian function, see http://www.iec.northwestern.edu/Music/electrostatic/electrostatic.htm) for the Ewald method	15, 6.7
xyz dimensions of the system	51.338, 51.338, 51.338
Angles of the unit cell (º)	90.0, 90.0, 90.0

3. Additional details for constant temperature molecular dynamics of gold nanoclusters in IRMOF-1 at ambient temperature

Software	MuSiC[3]
Number of time steps	10000000
Time step, ps	0.0002
Integrator	Gear predictor-corrector
Thermostat	Nose-Hoover
Thermostat parameter, Q_{nose} (kcal/mol)	1000
Iterations used for statistical sampling	50%
Temperature, K	300

4. Structure of the Au13 cluster and partial charges from the Mulliken analysis[4]

Atom number	x	y	z	Type	q, e
1	0	0	0	Au	-0.012
2	2.81675	-0.06406	-0.55608	Au	-0.012
3	0.740504	-0.35438	-2.5232	Au	0.144

4	3.442945	-0.49098	-3.14435	Au	-0.012
5	2.209357	1.941327	-2.3734	Au	-0.012
6	-2.0049	-0.2429	-1.92655	Au	-0.012
7	-0.72809	-2.65219	-2.7371	Au	-0.012
8	1.293648	-2.43921	-0.77963	Au	-0.012
9	-1.21937	-0.62952	-4.54356	Au	-0.012
10	0.289067	1.682068	-4.41479	Au	-0.012
11	-0.52443	2.085102	-1.79024	Au	-0.012
12	1.504473	-0.7197	-5.1262	Au	-0.012
13	1.970518	-2.81983	-3.44875	Au	-0.012

5. Structural characteristics of all systems, considered in this work

	Reference perfect crystal	Percentage of the linkers removed						System with a 20Å mesopore	System with residual DMF	System with gold nanoclusters
		5	10	20	50	65	73			
Density g/cm^3	0.604	0.593	0.581	0.558	0.481	0.423	0.287	0.428	0.625	0.762
Volume (He) cm^3/g	1.358	1.384	1.413	1.472	1.713	1.972	3.089	2.028	1.267	1.053
Surface area (m^2/cm^3)	2043.91	2046.52	2066.93	2088.48	2137.96	2041.04	1457.04	1519.49	2026.6	2040.11
Surface area (m^2/g)	3381.49	3448.83	3556.78	3744.09	4446.09	4820.02	5084.12	3719.05	3242.3	2678.84
Pore limiting diameter (Å)	7.71	7.71	7.71	7.71	8.84	9.93	16.63	21.41	7.52	7.65
D_{max} (Å)	14.95	14.95	14.95	14.95	16.84	19.4	25.67	24.58	14.71	14.85

1. **A. K. Rappe, C. J. Casewit, K. S. Colwell, W. A. Goddard and W. M. Skiff, *Journal of the American Chemical Society*, 1992, 114, 10024-10035.**
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3. **A. Gupta, S. Chempath, M. J. Sanborn, L. A. Clark and R. Q. Snurr, *Molecular Simulation*, 2003, 29, 29-46.**
4. **X. Zhang, C. Q. Sun and H. Hirao, *Physical Chemistry Chemical Physics*, 2013, 15, 19284-19292.**