

# **Dyfuzja gazów szlachetnych w nanoporach materiałów węglowych**

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**KONFERENCJĘ UŻYTKOWNIKÓW KDM 2017**

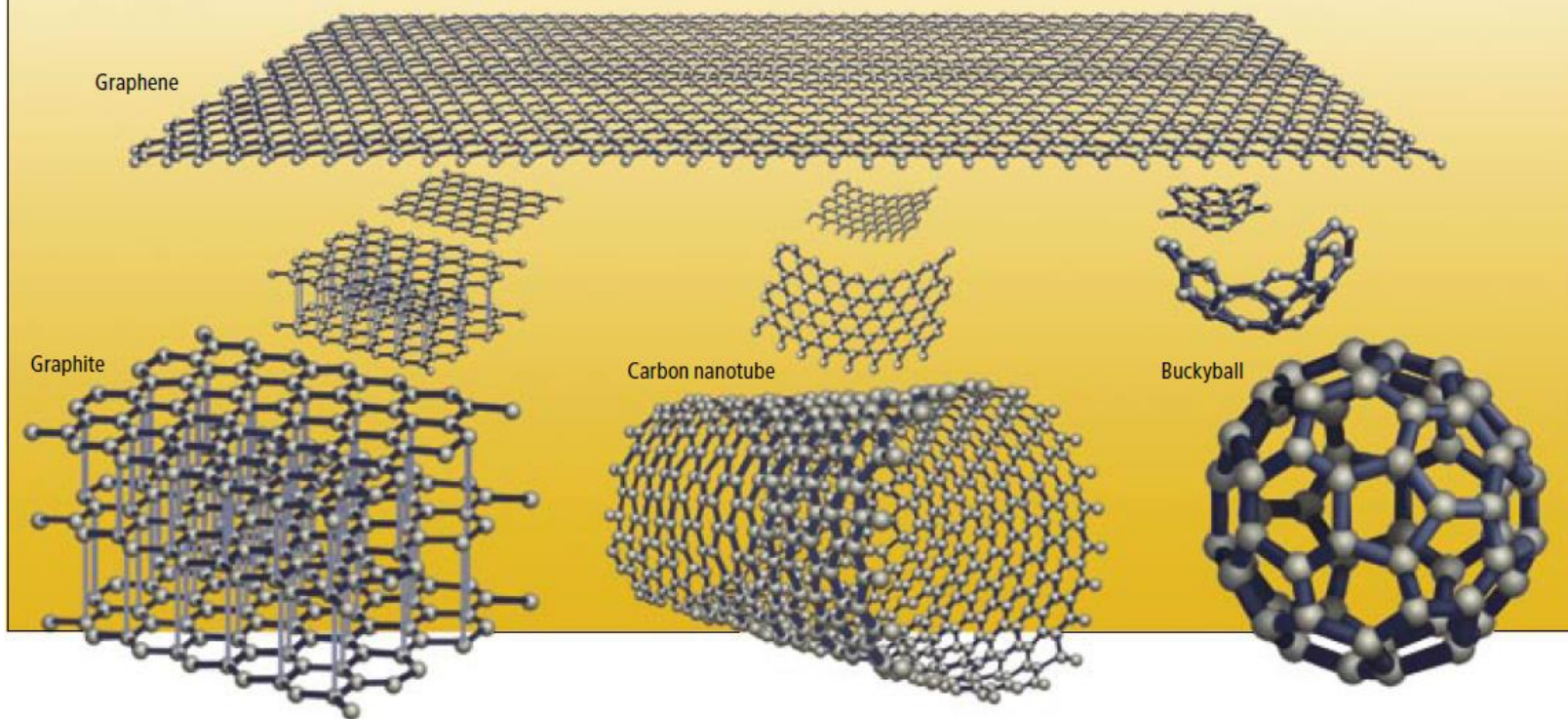
**„Nowe trendy w użytkowaniu KDM”**

[MOLECULAR FORMS]

## THE MOTHER OF ALL GRAPHITES

Graphene (*below, top*), a plane of carbon atoms that resembles chicken wire, is the basic building block of all the "graphitic" materials depicted below. Graphite (*bottom row at left*), the main component of pencil "lead," is a crumbly substance that resembles a layer cake of weakly bonded

graphene sheets. When graphene is wrapped into rounded forms, fullerenes result. They include honeycombed cylinders known as carbon nanotubes (*bottom row at center*) and soccer ball-shaped molecules called buckyballs (*bottom row at right*), as well as various shapes that combine the two forms.





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Guest Editorial

## Nomenclature of $sp^2$ carbon nanoforms

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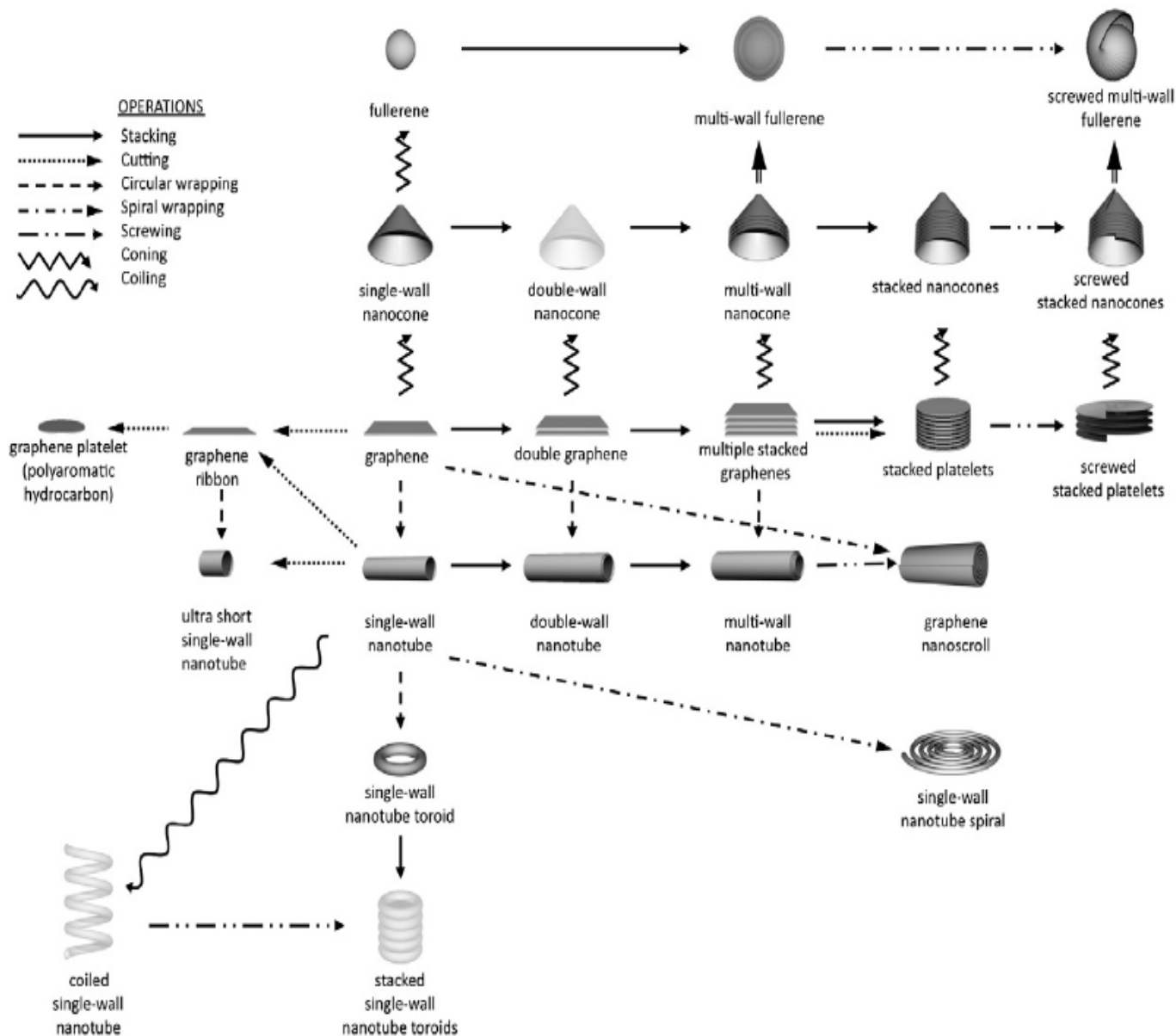
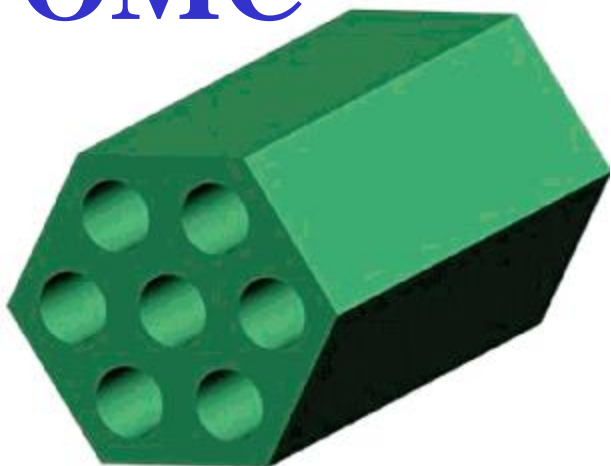


Fig. 2 – “Family tree” of primary carbon nanoforms showing the topological relationships between them. We note that all 1D forms can undergo the same operations as for the single-walled nanotube. For each form further operations are also possible such as polygonisation (see text). In addition hybrid forms (such as fullerene-filled nanotubes) are not included. Forms which have not been identified experimentally are faded. A description of each operation can be found in the text.

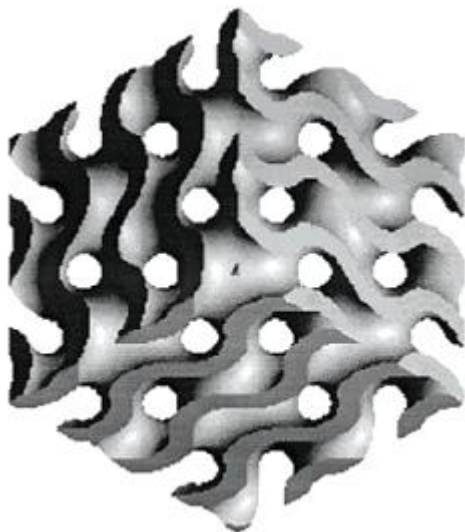


# OMC



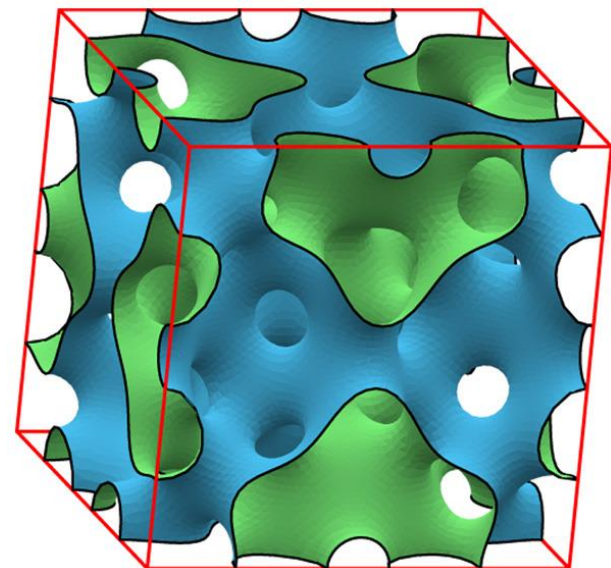
*p6mm*

**SBA-15**



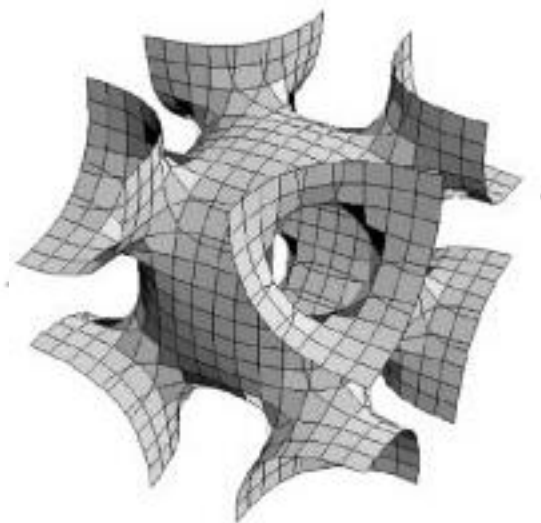
*Ia3d,*

**MCM-48**



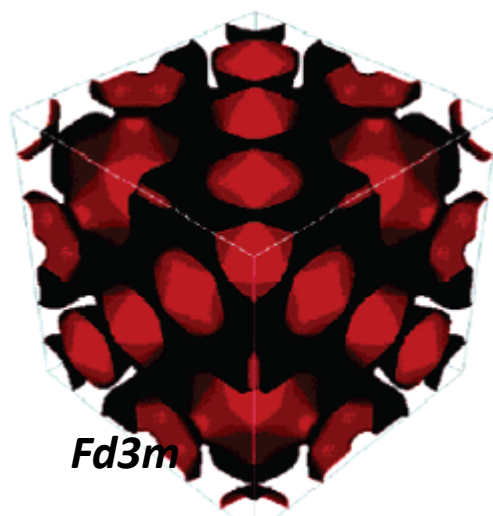
*Pm3n*

**SBA-1 and 6**



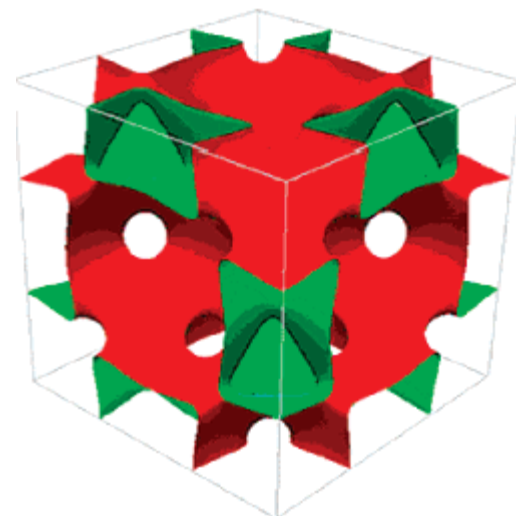
*Im3m*

**SBA-16**



*Fd3m*

**FDU-2**



*Fm3m.*

**KIT-5**

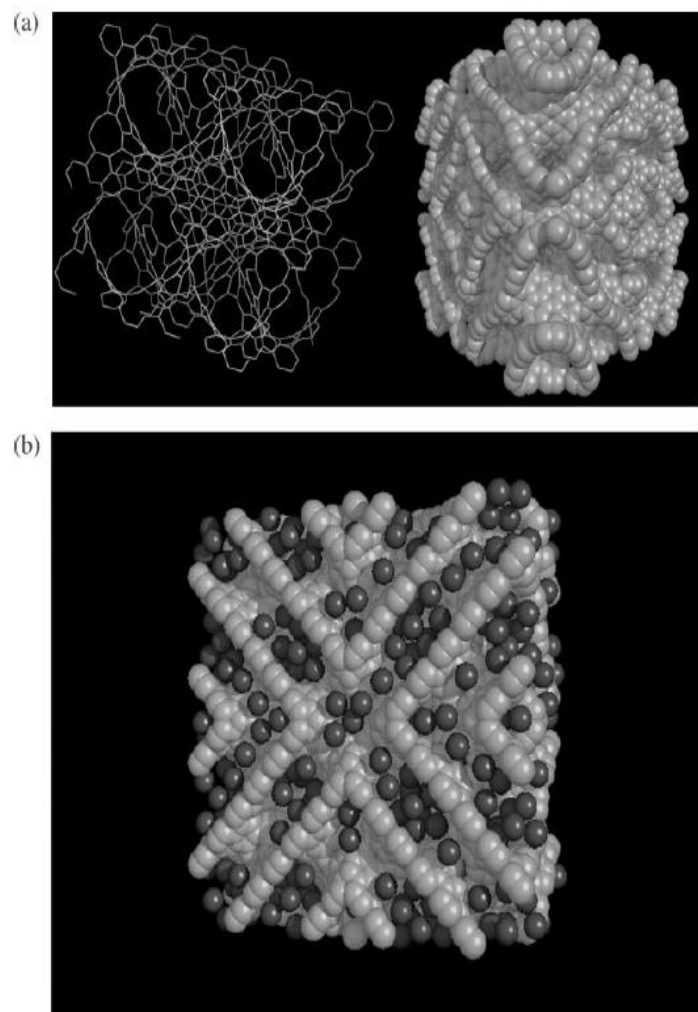
# Hydrogen storage in nanoporous carbon materials: myth and facts

Piotr Kowalczyk,<sup>a</sup> Robert Hołyst,<sup>a</sup> Mauricio Terrones<sup>b</sup> and Humberto Terrones<sup>b</sup>

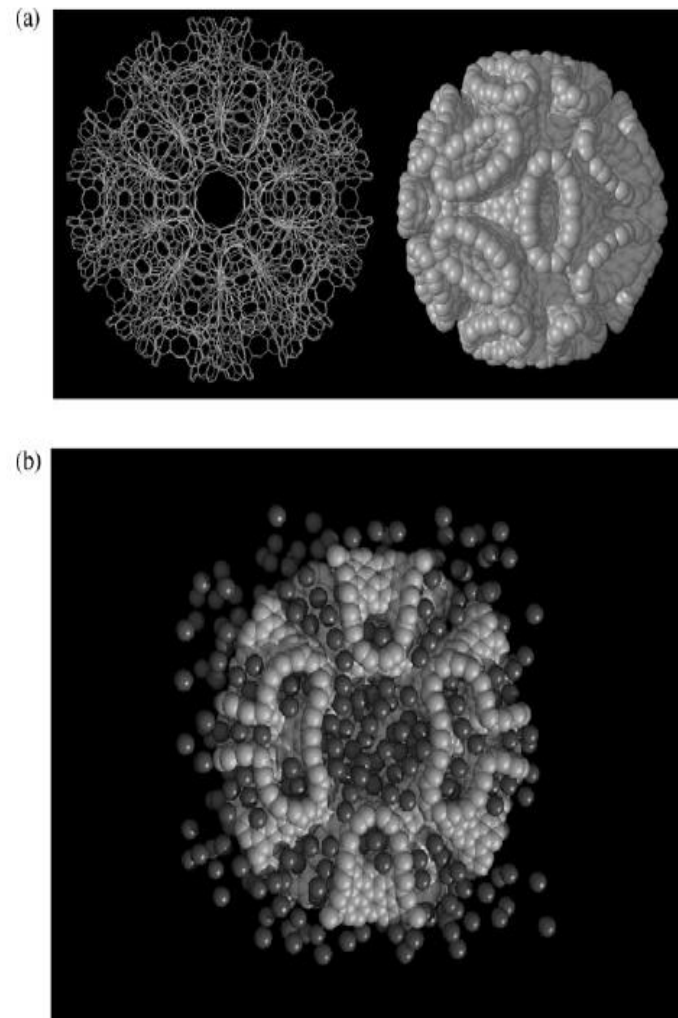
*Received 22nd December 2006, Accepted 9th March 2007*

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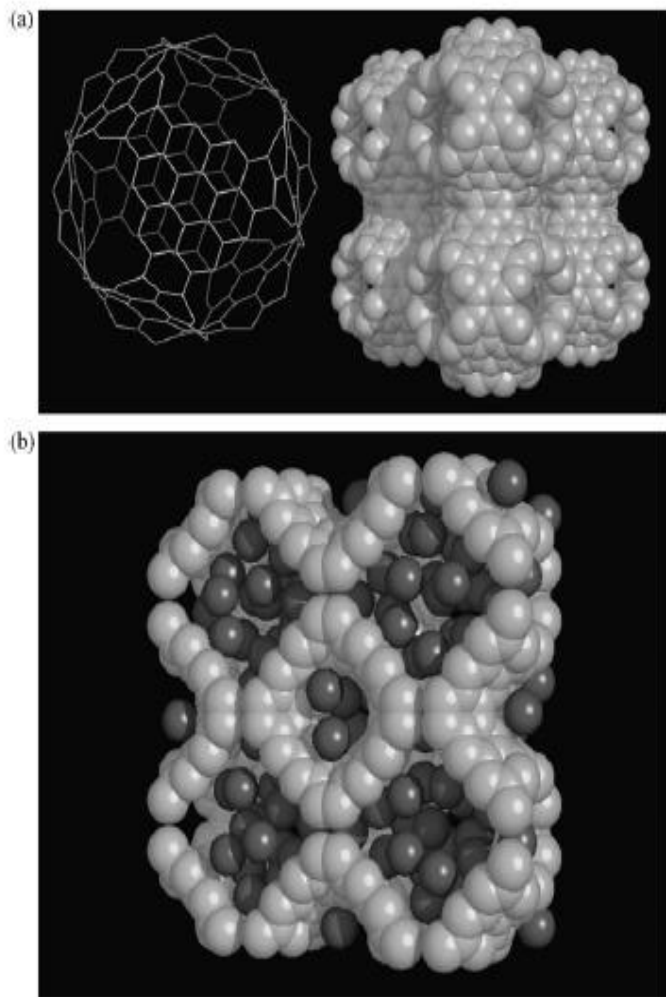
DOI: 10.1039/b618747a



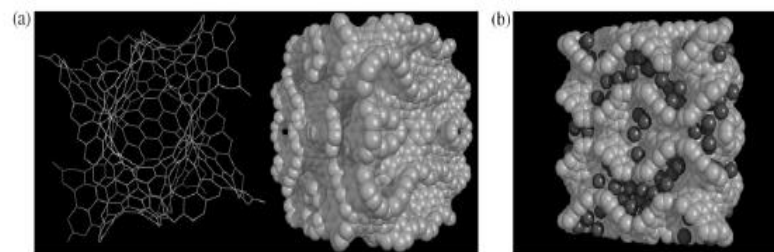
**Fig. 5** (a) Diamond carbon nanoporous material. Left image shows carbon rings on the surface and right image shows eight unit cells of the structure decorated by carbon atoms. (b) A snapshot of hydrogen adsorbed in the diamond nanoporous carbon material at 3.8 MPa and 77 K collected from the simulation (cross-section is shown).



**Fig. 4** (a) The quasi-periodic icosahedral nanoporous carbon material. Left figure shows carbon rings on the surface and right figure shows eight unit cells of the structure decorated by carbon atoms. (b) A snapshot of hydrogen adsorbed in the quasi-periodic icosahedral nanoporous carbon material at 3.8 MPa and 77 K.



**Fig. 6** (a) Primitive carbon nanoporous material. Left image shows carbon rings on the surface and right image shows eight unit cells of the structure decorated by carbon atoms. (b) A snapshot of hydrogen adsorbed in the primitive nanoporous carbon material at 3.8 MPa and 77 K collected from the simulation (cross section is shown).



**Fig. 7** (a) Gyroid carbon nanoporous material. Left image shows carbon rings on the surface and right image shows eight unit cells of the structure decorated by carbon atoms. (b) A snapshot of hydrogen adsorbed in the gyroid nanoporous carbon material at 3.8 MPa and 77 K collected from the FH-GCMC simulation (cross section of the material).



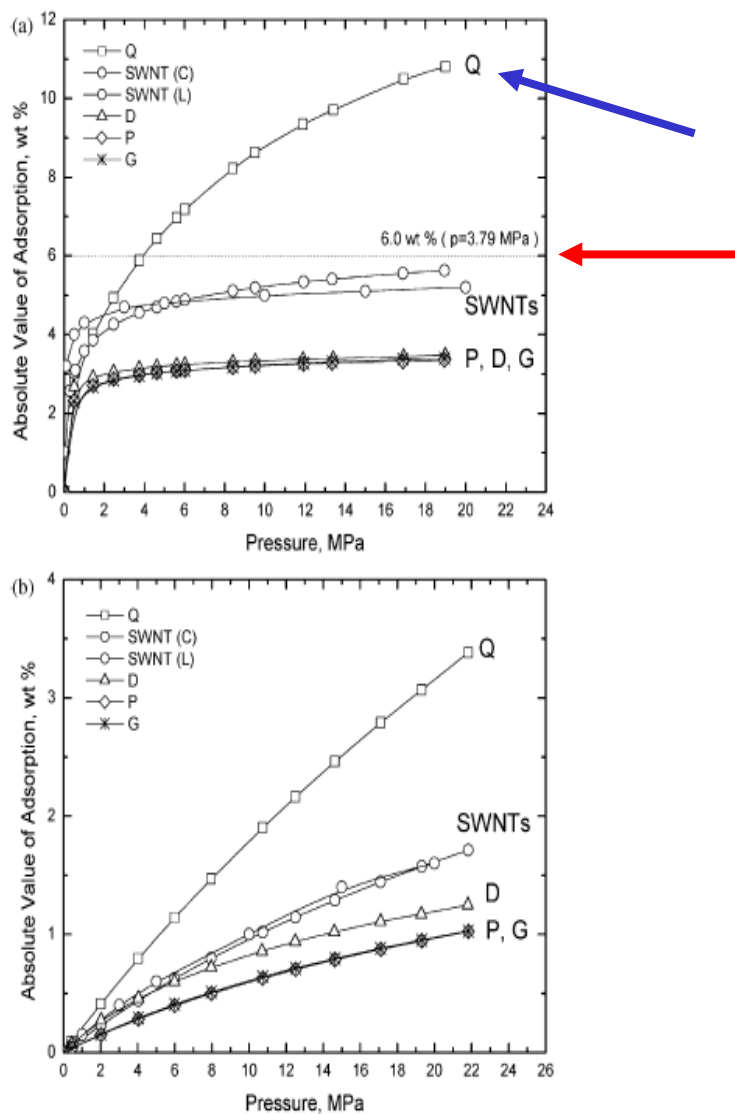


Fig. 1 (a) Simulated absolute value of adsorption (hydrogen gravimetric weight percent) at 77 K from the computer simulations. Abbreviations: Q – quasi-periodic icosahedral nanoporous carbon material, SWNT (C) – hexagonal bundle of SWNTs, SWNT (L) – simulation results of hydrogen storage in SWNTs (single wall carbon nanotubes) taken from Levesque *et al.*<sup>16</sup> for comparison with our results, D – diamond nanoporous carbon material, P – primitive nanoporous carbon material, and G – gyroid nanoporous carbon material. (b) Same at 303 K.

# Periodic Table of the Elements

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1 IA 11A H Hydrogen 1.008																	18 VIIIA 8A He Helium 4.003						
3 Li Lithium 6.941	4 Be Beryllium 9.012																	13 IIIA 3A B Boron 10.811	14 IVA 4A C Carbon 12.011	15 VA 5A N Nitrogen 14.007	16 VIA 6A O Oxygen 15.999	17 VIIA 7A F Fluorine 18.998	18 Ne Neon 20.180
11 Na Sodium 22.990	12 Mg Magnesium 24.305	3 IIIB 3B	4 IVB 4B	5 VB 5B	6 VIB 6B	7 VIIB 7B	8 VIII 8	9 VIII 8	10 VIII 8	11 IB 1B	12 IIB 2B	13 Al Aluminum 26.982	14 Si Silicon 28.086	15 P Phosphorus 30.974	16 S Sulfur 32.066	17 Cl Chlorine 35.453	18 Ar Argon 39.948						
19 K Potassium 39.098	20 Ca Calcium 40.078	21 Sc Scandium 44.956	22 Ti Titanium 47.88	23 V Vanadium 50.942	24 Cr Chromium 51.996	25 Mn Manganese 54.938	26 Fe Iron 55.933	27 Co Cobalt 58.933	28 Ni Nickel 58.693	29 Cu Copper 63.546	30 Zn Zinc 65.39	31 Ga Gallium 69.732	32 Ge Germanium 72.61	33 As Arsenic 74.922	34 Se Selenium 78.09	35 Br Bromine 79.904	36 Kr Krypton 84.80						
37 Rb Rubidium 84.468	38 Sr Strontium 87.62	39 Y Yttrium 88.906	40 Zr Zirconium 91.224	41 Nb Niobium 92.906	42 Mo Molybdenum 95.94	43 Tc Technetium 98.907	44 Ru Ruthenium 101.07	45 Rh Rhodium 102.906	46 Pd Palladium 106.42	47 Ag Silver 107.868	48 Cd Cadmium 112.411	49 In Indium 114.818	50 Sn Tin 118.71	51 Sb Antimony 121.760	52 Te Tellurium 127.6	53 I Iodine 126.904	54 Xe Xenon 131.29						
55 Cs Cesium 132.905	56 Ba Barium 137.327	57-71	72 Hf Hafnium 178.49	73 Ta Tantalum 180.948	74 W Tungsten 183.85	75 Re Rhenium 186.207	76 Os Osmium 190.23	77 Ir Iridium 192.22	78 Pt Platinum 195.08	79 Au Gold 196.967	80 Hg Mercury 200.59	81 Tl Thallium 204.383	82 Pb Lead 207.2	83 Bi Bismuth 208.980	84 Po Polonium [208.982]	85 At Astatine 209.987	86 Rn Radon 222.018						
87 Fr Francium 223.020	88 Ra Radium 226.025	89-103	104 Rf Rutherfordium [261]	105 Db Dubnium [262]	106 Sg Seaborgium [266]	107 Bh Bohrium [264]	108 Hs Hassium [269]	109 Mt Meitnerium [268]	110 Ds Darmstadtium [269]	111 Rg Roentgenium [272]	112 Cn Copernicium [277]	113 Uut Ununtrium unknown	114 Fl Flerovium [289]	115 Uup Ununpentium unknown	116 Lv Livermorium [298]	117 Uus Ununseptium unknown	118 Uuo Ununoctium unknown						

Lanthanide Series

57 <b>La</b> Lanthanum 138.906	58 <b>Ce</b> Cerium 140.115	59 <b>Pr</b> Praseodymium 140.908	60 <b>Nd</b> Neodymium 144.24	61 <b>Pm</b> Promethium 144.913	62 <b>Sm</b> Samarium 150.36	63 <b>Eu</b> Europium 151.966	64 <b>Gd</b> Gadolinium 157.25	65 <b>Tb</b> Terbium 158.925	66 <b>Dy</b> Dysprosium 162.50	67 <b>Ho</b> Holmium 164.930	68 <b>Er</b> Erbium 167.26	69 <b>Tm</b> Thulium 168.934	70 <b>Yb</b> Ytterbium 173.04	71 <b>Lu</b> Lutetium 174.967
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Actinide Series

89 <b>Ac</b> Actinium 227.028	90 <b>Th</b> Thorium 232.038	91 <b>Pa</b> Protactinium 231.036	92 <b>U</b> Uranium 238.029	93 <b>Np</b> Neptunium 237.048	94 <b>Pu</b> Plutonium 244.064	95 <b>Am</b> Americium 243.061	96 <b>Cm</b> Curium 247.070	97 <b>Bk</b> Berkelium 247.070	98 <b>Cf</b> Californium 251.080	99 <b>Es</b> Einsteinium [254]	100 <b>Fm</b> Fermium 257.095	101 <b>Md</b> Mendelevium 258.1	102 <b>No</b> Nobelium 259.101	103 <b>Lr</b> Lawrencium [262]
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Alkali Metal	Alkaline Earth	Transition Metal	Semimetal	Nonmetal	Basic Metal	Halogen	Noble Gas	Lanthanide	Actinide
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**Helium is a rare gas with a wide range of applications**

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Similarly, resources of He (e.g., natural gas, air, and waste gases of ammonia synthesis) **are composed of various small particles** (such as  $\text{CH}_4$ ,  $\text{CO}$ ,  $\text{Ar}$ ,  $\text{Ne}$ ,  $\text{O}_2$ , and others) **that need to be removed through purification processes.**

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**The main aim: looking for new carbon materials!**

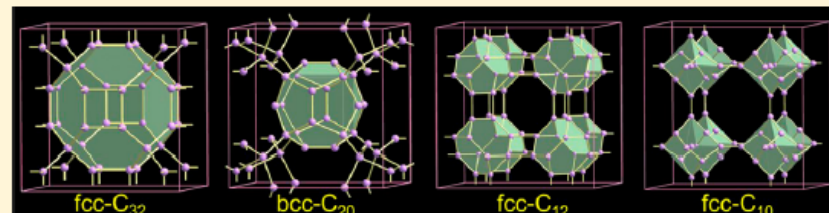
## Exotic Cubic Carbon Allotropes

Meng Hu,<sup>†</sup> Fei Tian,<sup>‡</sup> Zhisheng Zhao,<sup>†</sup> Quan Huang,<sup>†</sup> Bo Xu,<sup>†</sup> Li-Min Wang,<sup>†</sup> Hui-Tian Wang,<sup>‡</sup> Yongjun Tian,<sup>†</sup> and Julong He<sup>\*,†</sup>

<sup>†</sup>State Key Laboratory of Metastable Materials Science and Technology, Yanshan University, Qinhuangdao 066004, China

<sup>‡</sup>School of Physics and Key Laboratory of Weak-Light Nonlinear Photonics, Ministry of Education, Nankai University, Tianjin 300071, China

**ABSTRACT:** Elemental carbon exists in various aesthetically pleasing architectures. These forms include a group of synthesized allotropes with cubic modifications that have taken controversial or even unidentified crystal structures, which makes determining their physical properties difficult. In this study, four novel cubic carbon polymorphs (fcc-C<sub>10</sub>, fcc-C<sub>12</sub>, bcc-C<sub>20</sub>, and fcc-C<sub>32</sub>) that exhibit lattice parameters within the same range as those of undetermined cubic carbon allotropes are proposed by employing a newly developed ab initio particle-swarm optimization methodology for crystal structure prediction. The four structures are all three-dimensional polymers consisting of unique, small C<sub>10</sub>, C<sub>12</sub>, C<sub>20</sub>, and C<sub>32</sub> cages with quite low density. Investigation of their electronic and mechanical properties illustrate that the cage-like cubic carbons are all semiconductors with excellent mechanical performance, specifically superhardness and high ductility. Moreover, we readily explain a long-standing controversial experimentally synthesized cubic carbon (viz., the so-called “superdense” carbon) using the previously proposed bcc C<sub>6</sub> based on the coincident lattice constant and electron diffraction data between the theoretical and experimental results.

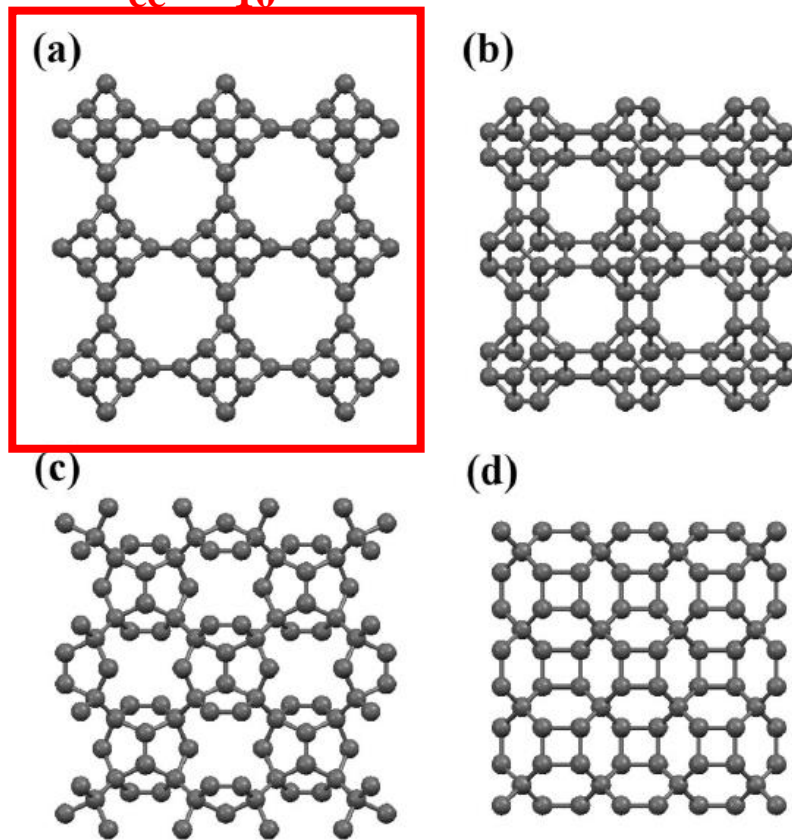


Cite this: *Phys. Chem. Chem. Phys.*, 2013, 15, 17366

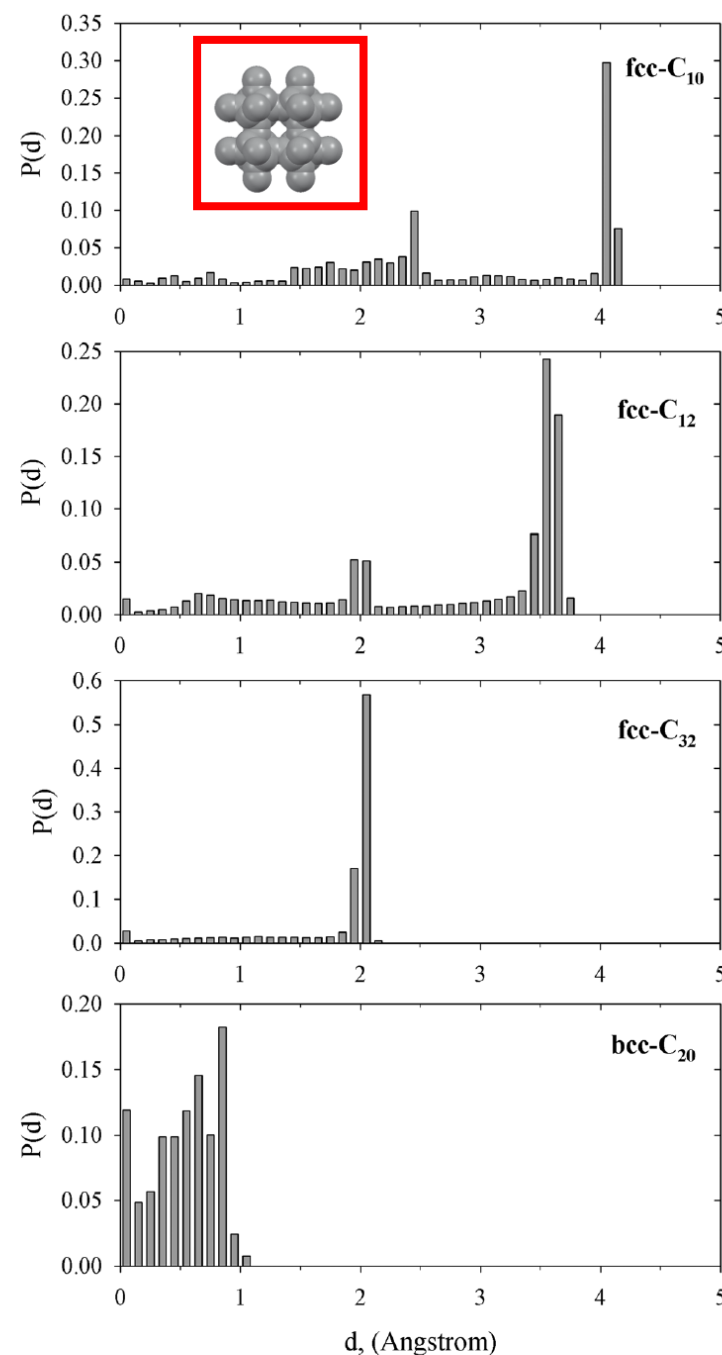
# To the pore and through and kinetics of helium in polymorphs†

Piotr Kowalczyk,<sup>\*a</sup> Julong He,<sup>b</sup> Meng and Artur P. Terzyk<sup>c</sup>

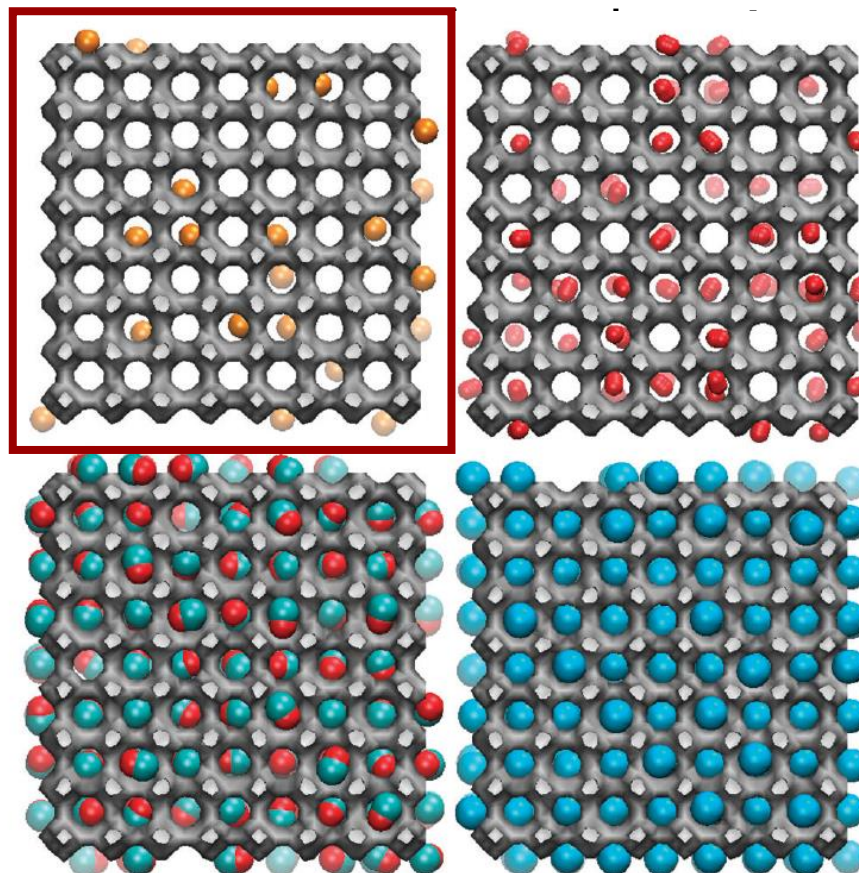
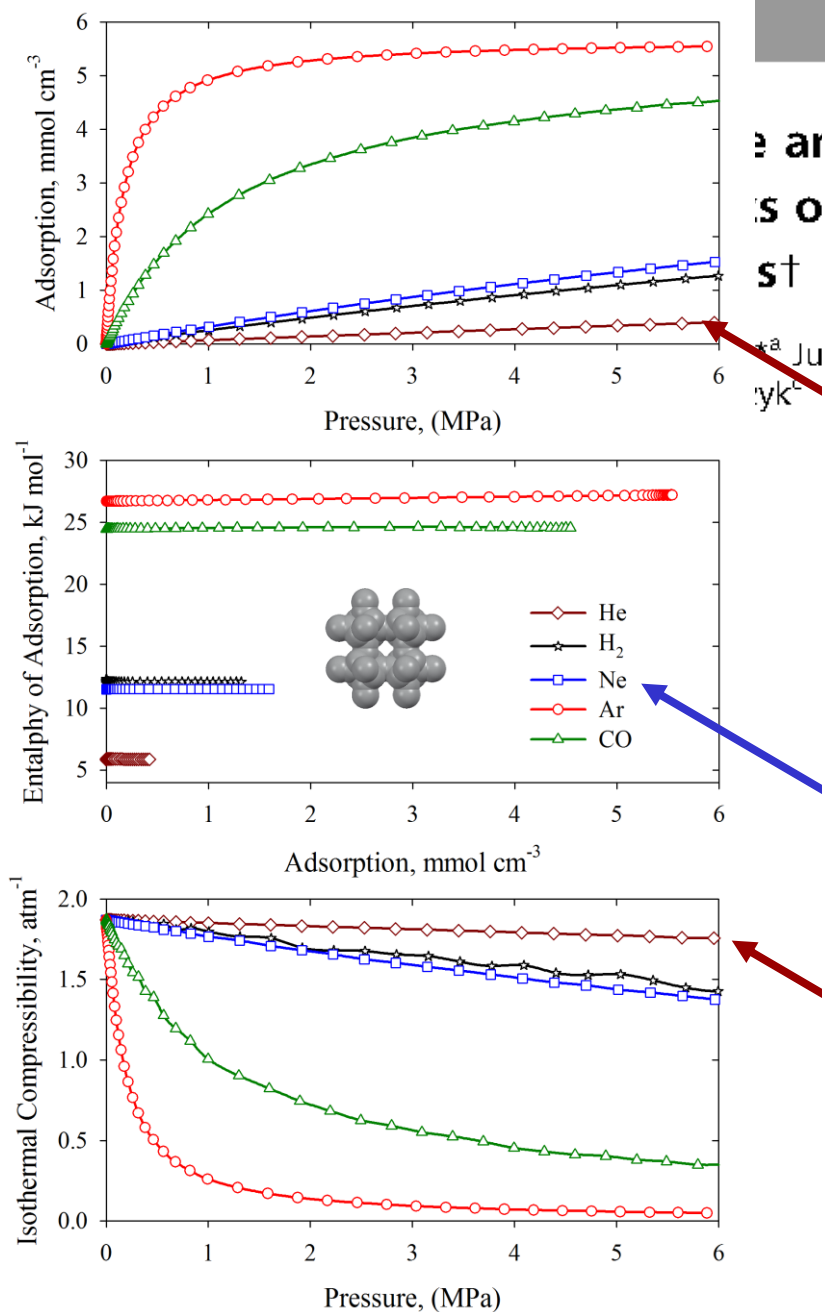
**f<sub>cc</sub>-C<sub>10</sub>**



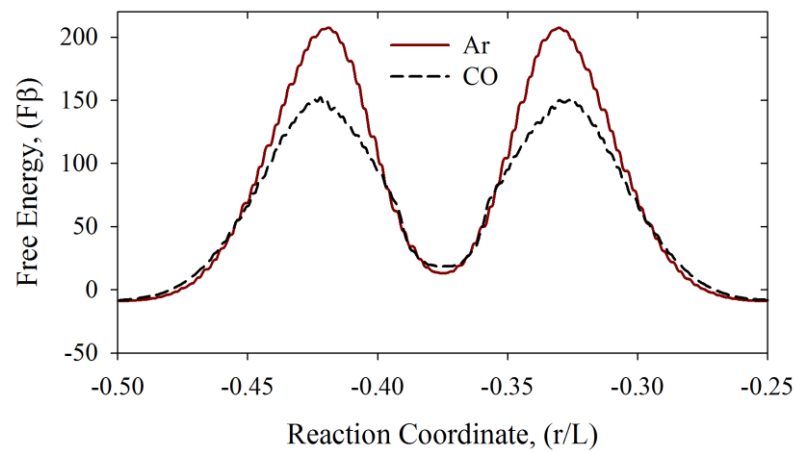
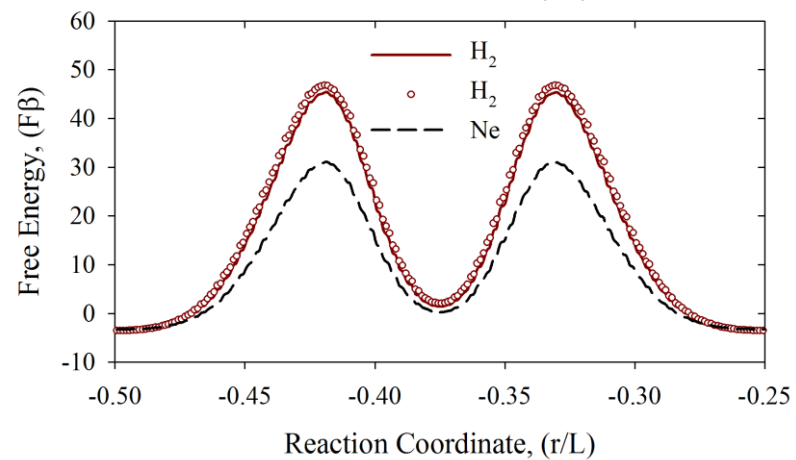
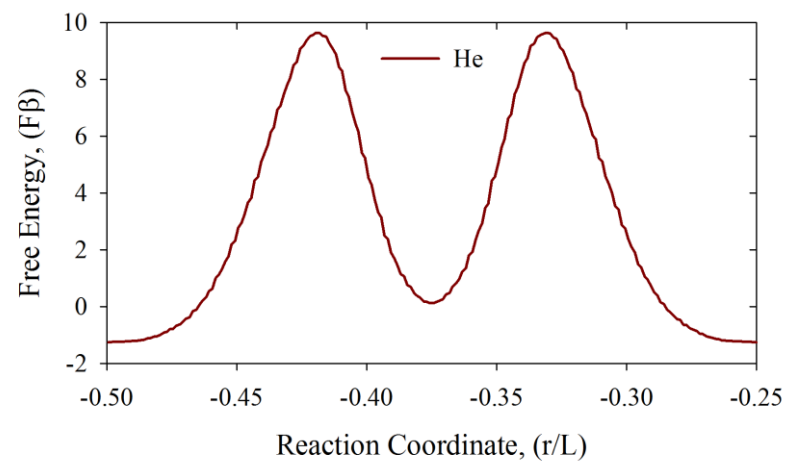
**Fig. 1** Crystal structures of the studied cubic carbon polymorphs:<sup>36</sup> (a) fcc-C<sub>10</sub>, (b) fcc-C<sub>12</sub>, (c) bcc-C<sub>20</sub>, and (d) fcc-C<sub>32</sub>.



**Fig. 3** Pore size distributions of the studied cubic carbon polymorphs computed from the method of Bhattacharya and Gubbins.<sup>37</sup>



**Fig. 5** GCMC snapshot of He, H<sub>2</sub>, CO, and Ar adsorbed in the fcc-C<sub>10</sub> cubic carbon crystal at 6 MPa and 298 K. Under the studied operating conditions, the fcc-C<sub>10</sub> cubic carbon crystal adsorbs 0.0017 g cm<sup>-3</sup> of He and 0.22 g cm<sup>-3</sup> of Ar (volumetric density of liquid He at 4.2 K and liquid Ar at 85.6 K are 0.147 g cm<sup>-3</sup> and 1.4 g cm<sup>-3</sup>, respectively).



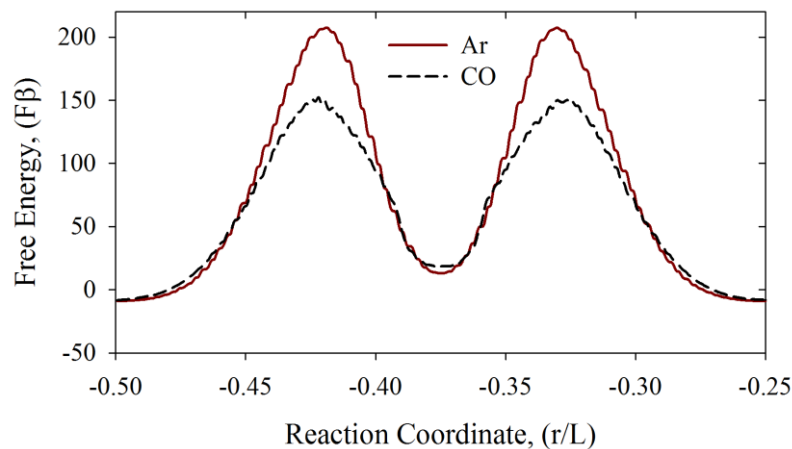
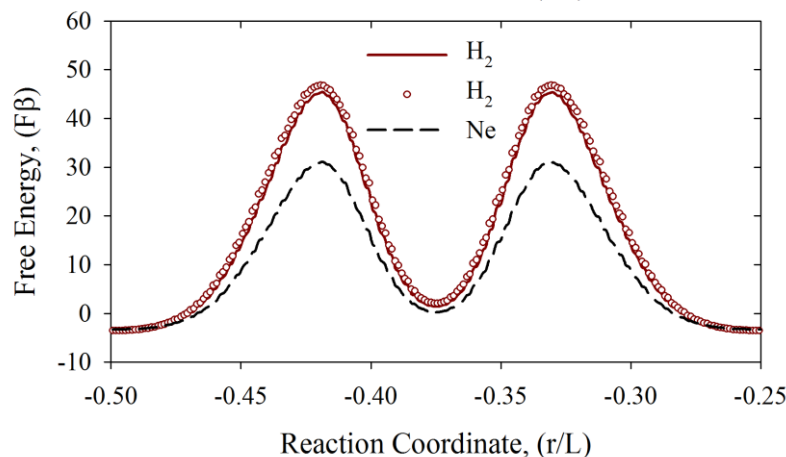
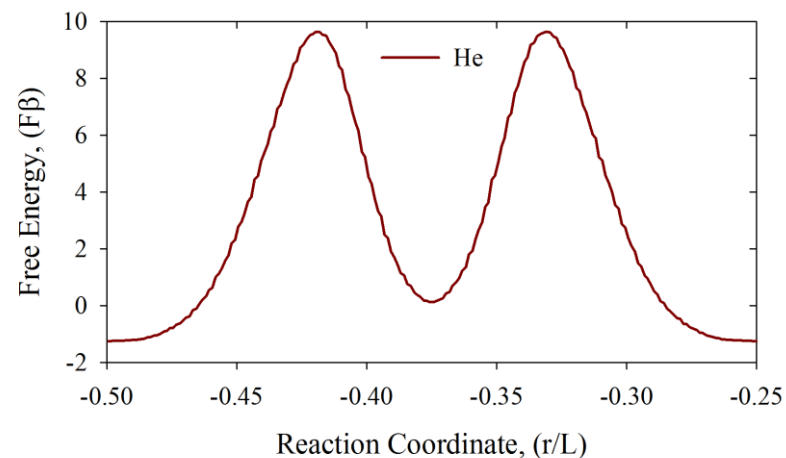


**Carbon cavities of fcc-C<sub>10</sub> carbon polymorph (with effective size of ~3.5-4 Å) are kinetically closed for common gaseous contaminants of helium fluid (including: Ne, Ar, H<sub>2</sub>, and CO).**

Because the sizes of nanowindows connecting carbon cavities are comparable with the effective size of He atom (~2.556 Å), we predicted a significant resistance for self-diffusion of He in fcc-C<sub>10</sub> crystal.

Computed self-diffusion coefficients  $\sim 1.3 \cdot 10^{-6} - 1.3 \cdot 10^{-7} \text{ cm}^2/\text{s}$  for He inside fcc-C<sub>10</sub> fall in the range characteristic for molecular diffusion in zeolites.

Infrequent “jumps” of He atoms between neighboring carbon cavities and kinetic rejection of other gaseous particles indicate potential application of fcc-C<sub>10</sub> carbon polymorph for kinetic molecular sieving of He near ambient temperatures.

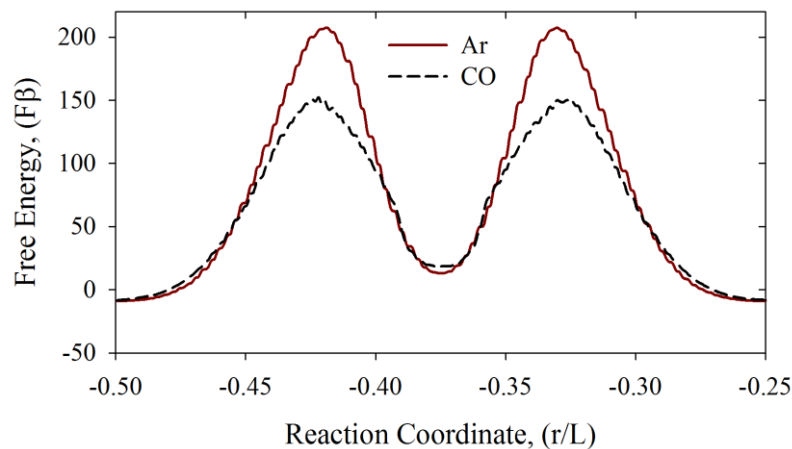
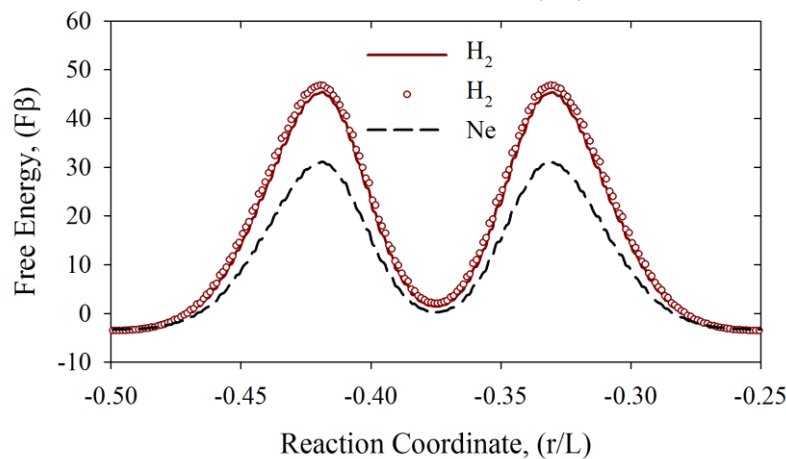
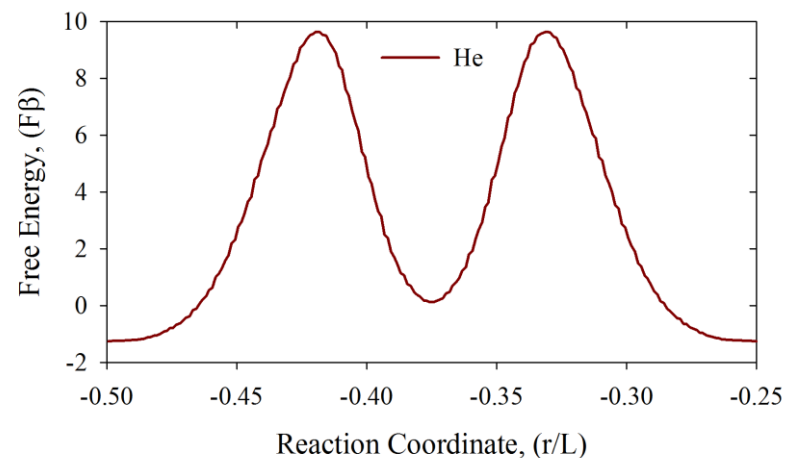


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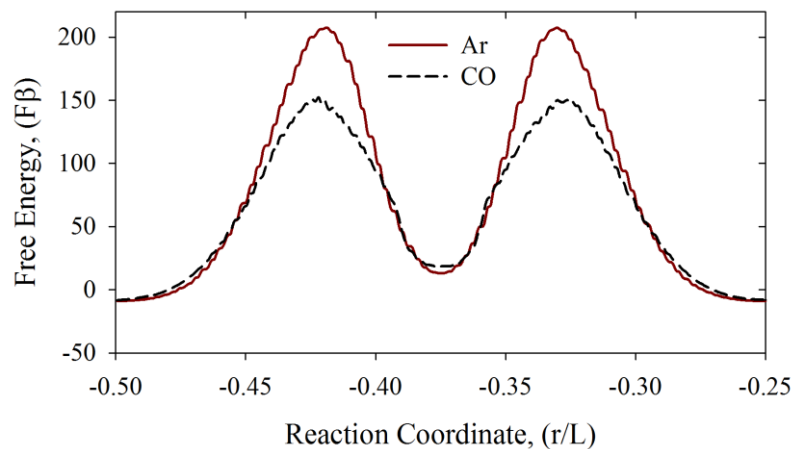
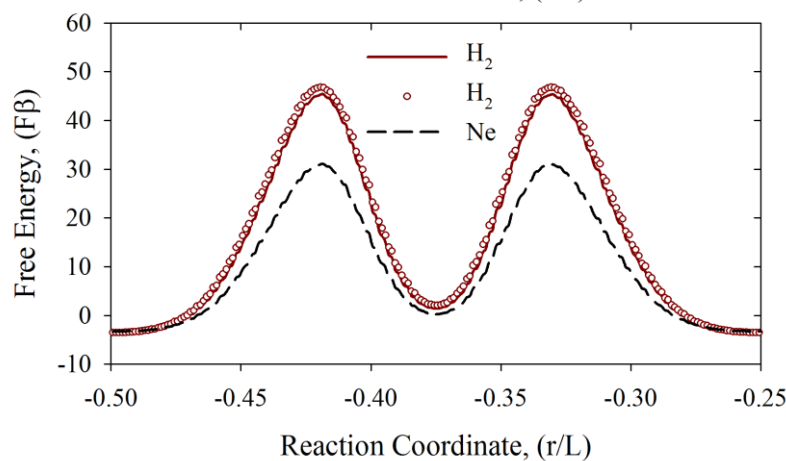
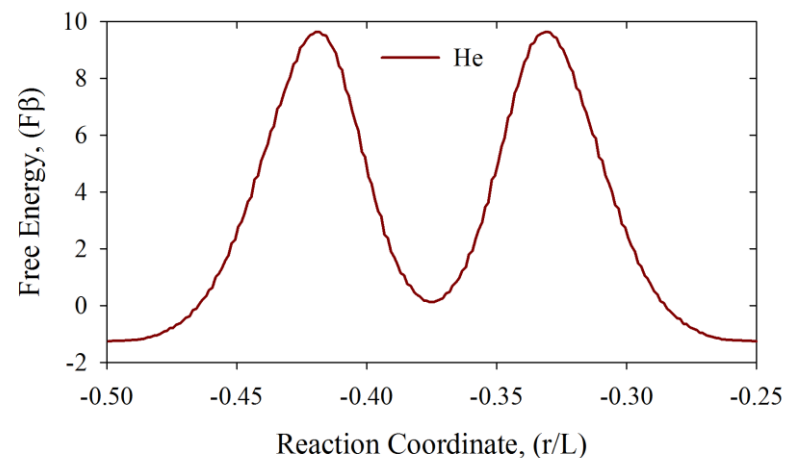


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**Computed self-diffusion coefficients ~ 1.3 10<sup>-6</sup> – 1.3 10<sup>-7</sup> cm<sup>2</sup>/s for He inside fcc-C<sub>10</sub> fall in the range characteristic for molecular diffusion in zeolites.**

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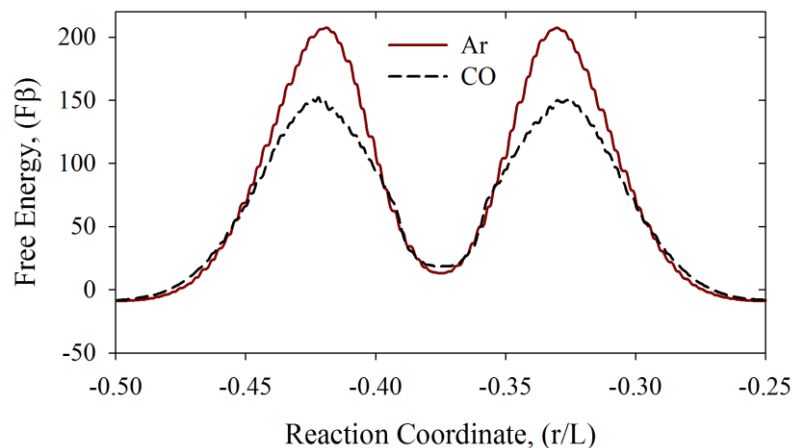
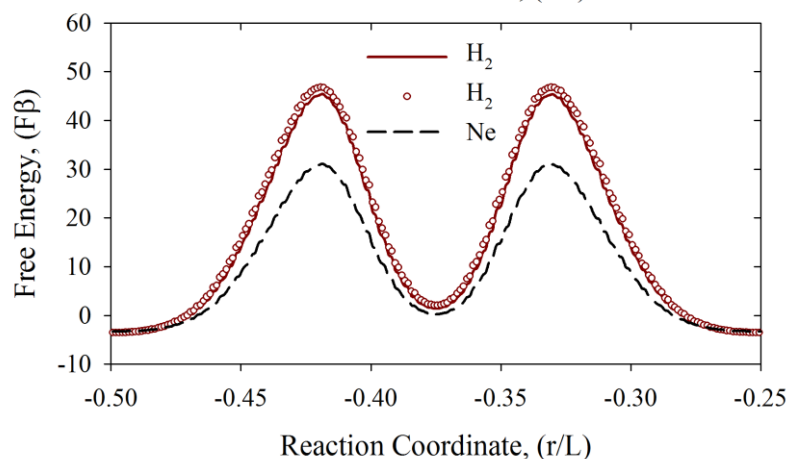
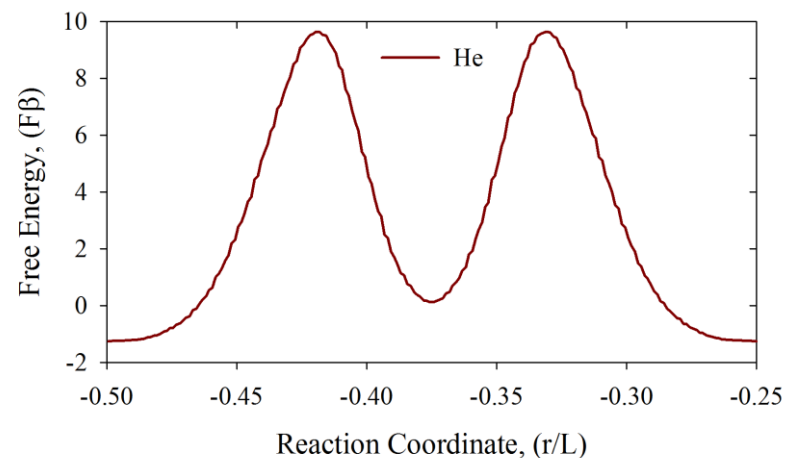


Carbon cavities of fcc-C<sub>10</sub> carbon polymorph (with effective size of  $\sim 3.5\text{-}4$  Å) are kinetically closed for common gaseous contaminants of helium fluid (including: Ne, Ar, H<sub>2</sub>, and CO).

Because the sizes of nanowindows connecting carbon cavities are comparable with the effective size of He atom ( $\sim 2.556$  Å), we predicted a significant resistance for self-diffusion of He in fcc-C<sub>10</sub> crystal.

Computed self-diffusion coefficients  $\sim 1.3 \cdot 10^{-6} - 1.3 \cdot 10^{-7} \text{ cm}^2/\text{s}$  for He inside fcc-C<sub>10</sub> fall in the range characteristic for molecular diffusion in zeolites.

**Infrequent “jumps” of He atoms between neighboring carbon cavities and kinetic rejection of other gaseous particles indicate potential application of fcc-C<sub>10</sub> carbon polymorph for kinetic molecular sieving of He near ambient temperatures.**



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87 Fr Francium 223.020	88 Ra Radium 226.025	89-103	104 Rf Rutherfordium [261]	105 Db Dubnium [262]	106 Sg Seaborgium [266]	107 Bh Bohrium [264]	108 Hs Hassium [269]	109 Mt Meitnerium [268]	110 Ds Darmstadtium [269]	111 Rg Roentgenium [272]	112 Cn Copernicium [277]	113 Uut Ununtrium unknown	114 Fl Flerovium [289]	115 Uup Ununpentium unknown	116 Lv Livermorium [298]	117 Uus Ununseptium unknown	118 Uuo Ununoctium unknown						

Lanthanide Series

57 <b>La</b> Lanthanum 138.906	58 <b>Ce</b> Cerium 140.115	59 <b>Pr</b> Praseodymium 140.908	60 <b>Nd</b> Neodymium 144.24	61 <b>Pm</b> Promethium 144.913	62 <b>Sm</b> Samarium 150.36	63 <b>Eu</b> Europium 151.966	64 <b>Gd</b> Gadolinium 157.25	65 <b>Tb</b> Terbium 158.925	66 <b>Dy</b> Dysprosium 162.50	67 <b>Ho</b> Holmium 164.930	68 <b>Er</b> Erbium 167.26	69 <b>Tm</b> Thulium 168.934	70 <b>Yb</b> Ytterbium 173.04	71 <b>Lu</b> Lutetium 174.967
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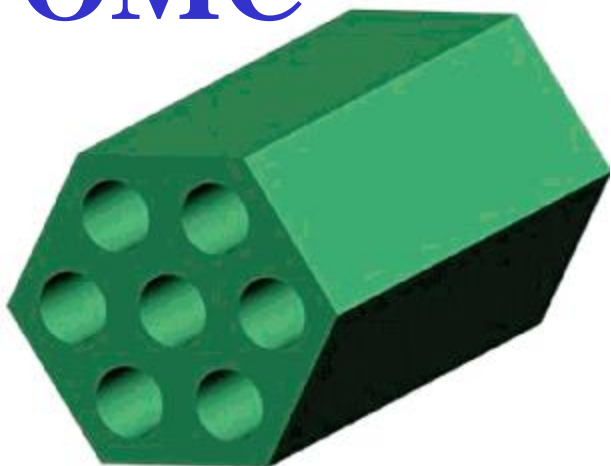
Actinide Series

89 <b>Ac</b> Actinium 227.028	90 <b>Th</b> Thorium 232.038	91 <b>Pa</b> Protactinium 231.036	92 <b>U</b> Uranium 238.029	93 <b>Np</b> Neptunium 237.048	94 <b>Pu</b> Plutonium 244.064	95 <b>Am</b> Americium 243.061	96 <b>Cm</b> Curium 247.070	97 <b>Bk</b> Berkelium 247.070	98 <b>Cf</b> Californium 251.080	99 <b>Es</b> Einsteinium [254]	100 <b>Fm</b> Fermium 257.095	101 <b>Md</b> Mendelevium 258.1	102 <b>No</b> Nobelium 259.101	103 <b>Lr</b> Lawrencium [262]
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Alkali Metal	Alkaline Earth	Transition Metal	Semimetal	Nonmetal	Basic Metal	Halogen	Noble Gas	Lanthanide	Actinide
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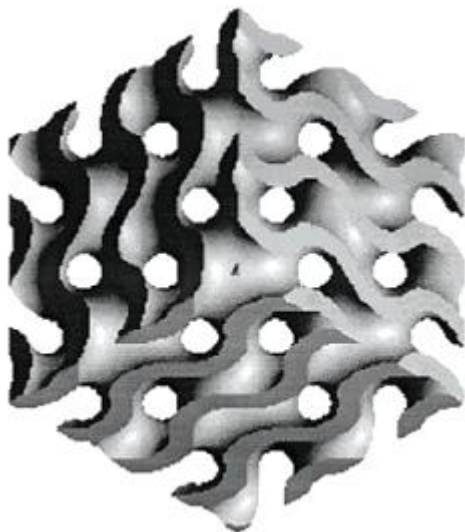


# OMC



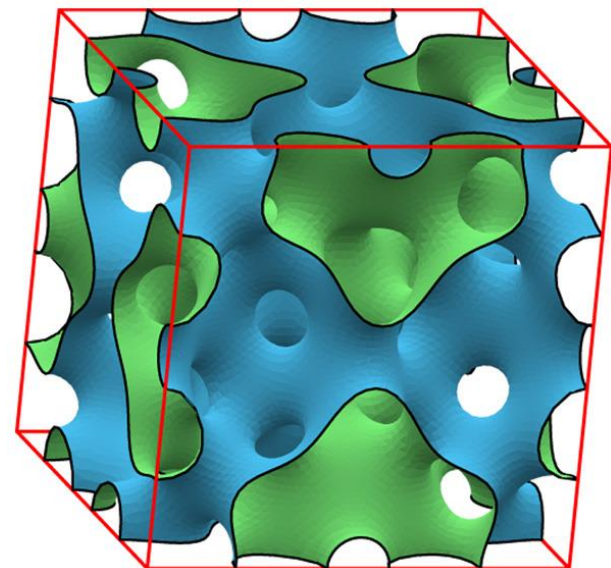
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**SBA-15**



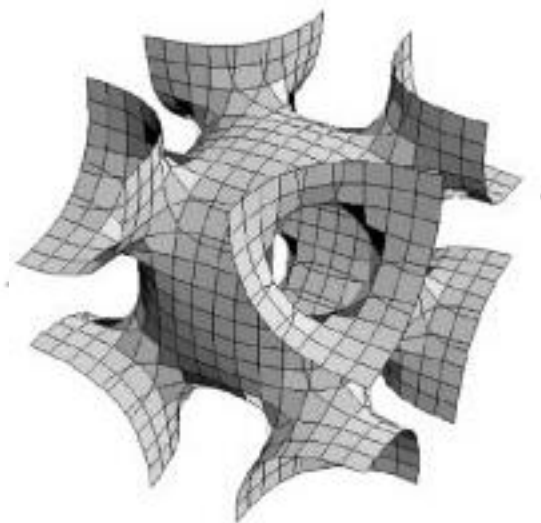
*Ia3d,*

**MCM-48**



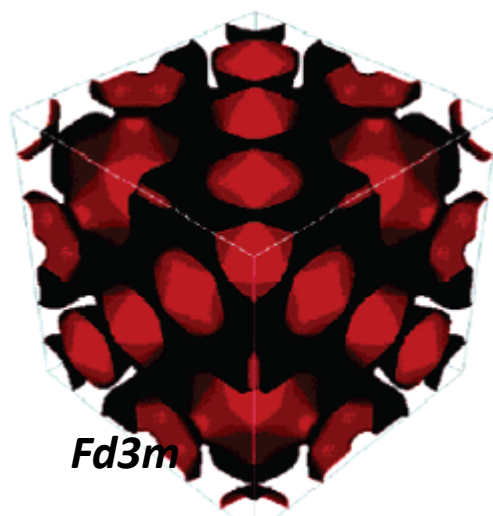
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**SBA-1 and 6**



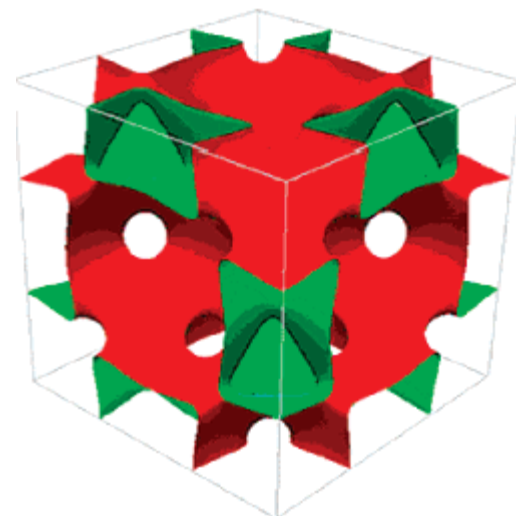
*Im3m*

**SBA-16**



*Fd3m*

**FDU-2**



**KIT-5**

*Fm3m.*



# Electrolyte Diffusion in Gyroidal Nanoporous Carbon

Adrien Nicolai, Joseph Monti, Colin Daniels, and Vincent Meunier\*

DOI: 10.1021/jp511919d

*J. Phys. Chem. C* 2015, 119, 2896–2903

Carbon 96 (2016) 998–1007



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journal homepage: [www.elsevier.com/locate/carbon](http://www.elsevier.com/locate/carbon)



Structural, energetic, and electronic properties of gyroidal graphene nanostructures



J.R. Owens<sup>a</sup>, C. Daniels<sup>a</sup>, A. Nicolai<sup>a</sup>, H. Terrones<sup>a</sup>, V. Meunier<sup>a, b, \*</sup>

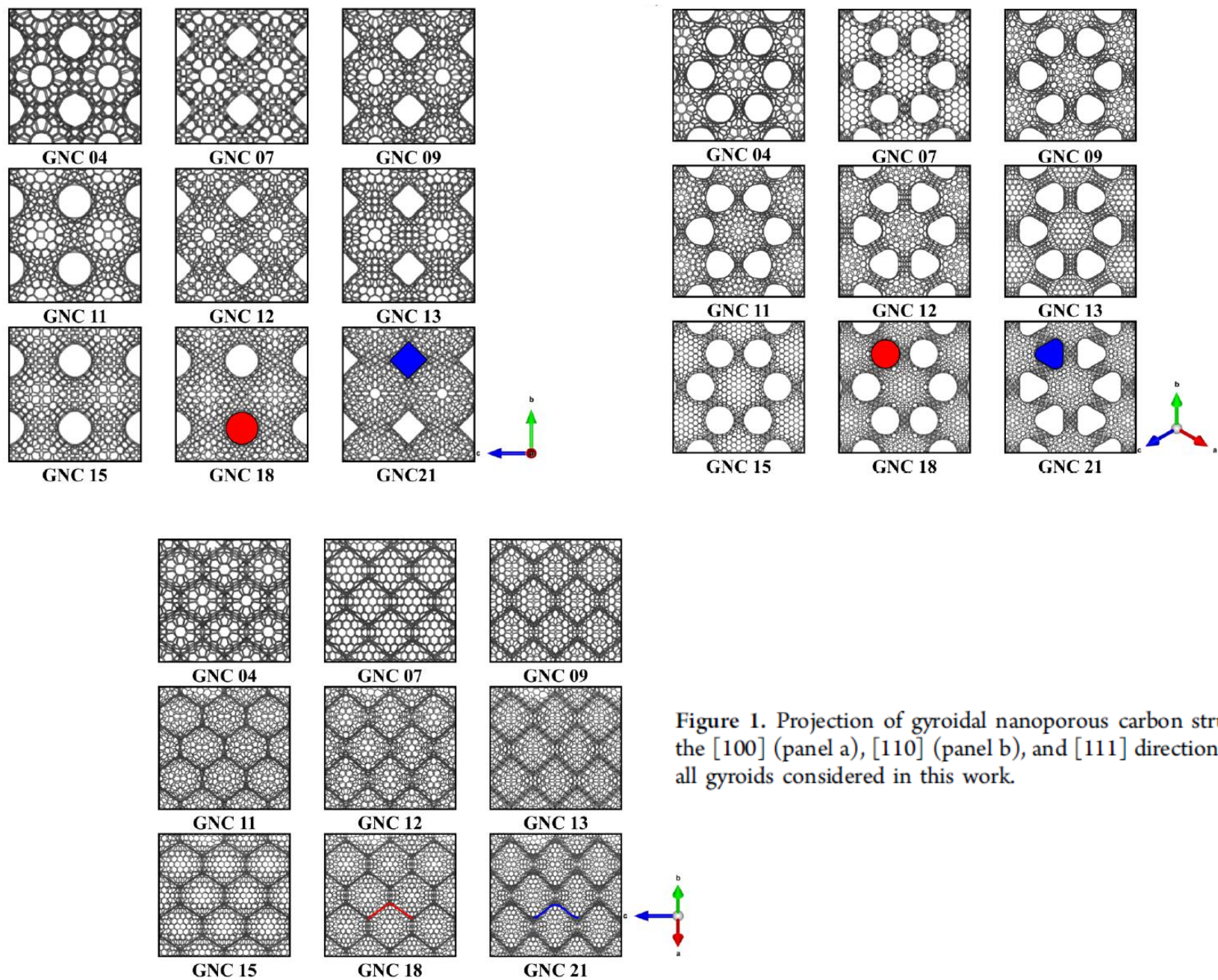
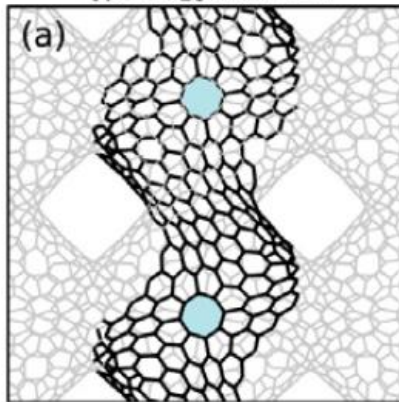
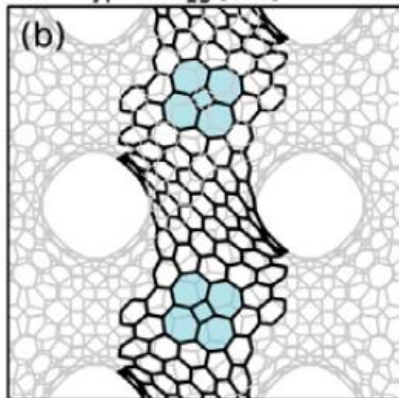


Figure 1. Projection of gyroidal nanoporous carbon structures along the  $[100]$  (panel a),  $[110]$  (panel b), and  $[111]$  direction (panel c) for all gyroids considered in this work.

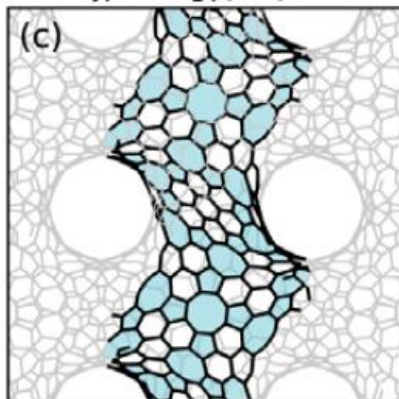
Type I:  $G_{16}$  [001] View



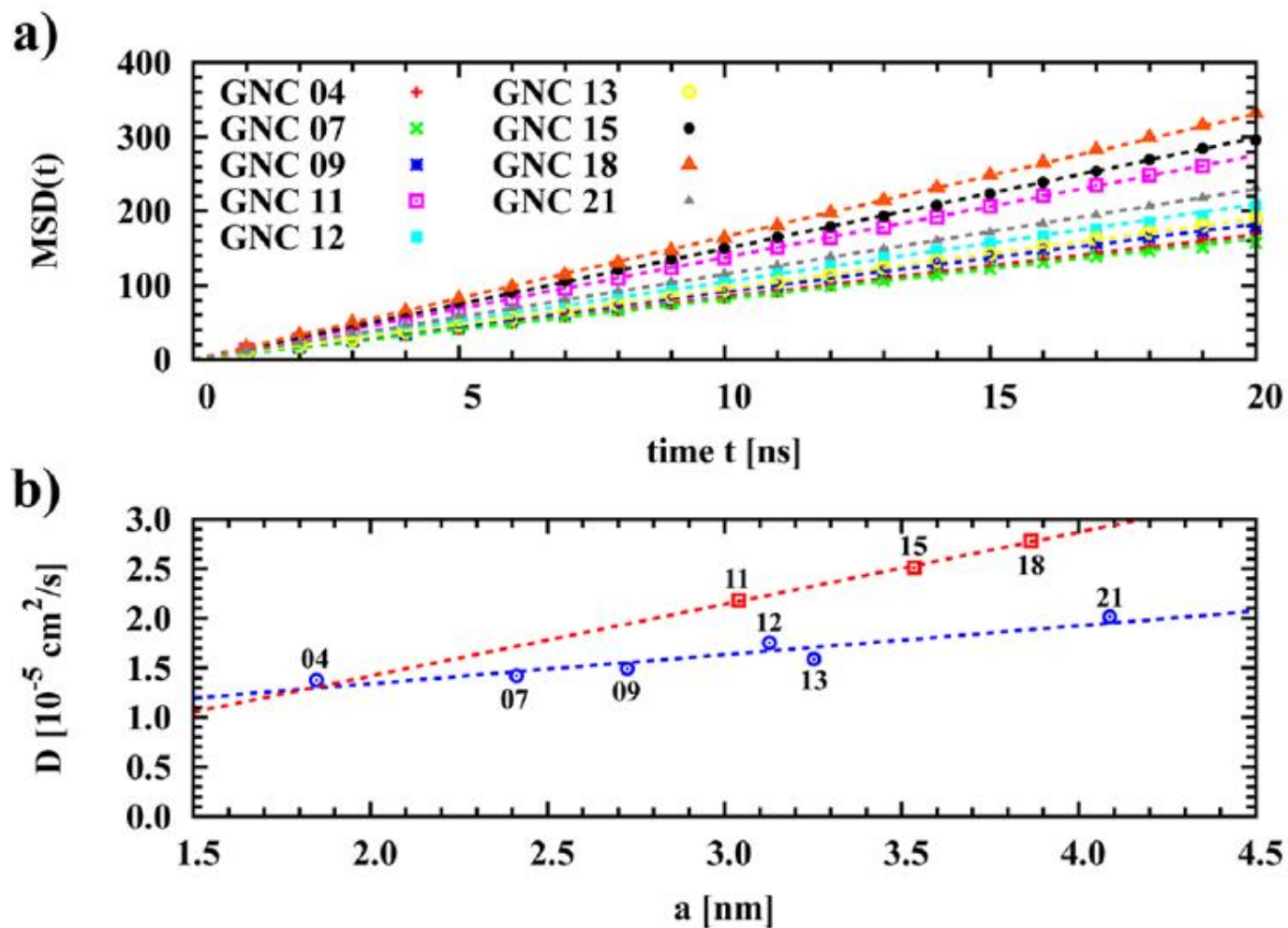
Type II:  $G_{15}$  [001] View



Type III:  $G_{14}$  [001] View







**Figure 3.** Diffusion properties of water in GNC structures. (a)  $\text{MSD}(t)$  of water molecules as a function of time computed from MD simulations. Points represent data extracted from MD simulations and lines the best-fit slope. (b) Self-diffusion coefficient  $D$  as a function of GNC unit cell parameter  $a$ . GNC indices are indicated for clarity. For comparison, the value of bulk TIP3P water using the same MD setup<sup>18</sup> is  $5.3 \times 10^{-5} \text{ cm}^2 \text{ s}^{-1}$ .

## **Gyroidal nanoporous carbons — Adsorption and separation properties explored using computer simulations\***

S. Furmaniak<sup>1</sup>, P.A. Gauden<sup>1</sup>, A.P. Terzyk<sup>1</sup>, P. Kowalczyk<sup>2</sup>

<sup>1</sup> Faculty of Chemistry, Physicochemistry of Carbon Materials Research Group,  
Nicolaus Copernicus University in Toruń, Gagarin St. 7, 87–100 Toruń, Poland

<sup>2</sup> School of Engineering and Information Technology, Murdoch University,  
Murdoch, Western Australia 6150, Australia

**CO<sub>2</sub>/CH<sub>4</sub>, CO<sub>2</sub>/N<sub>2</sub>, and CH<sub>4</sub>/N<sub>2</sub> mixtures**

# Gyroidal Nanoporous Carbon with Optimally Selective Neon Adsorption and Separation from Helium

**Piotr Kowalczyk<sup>\*1</sup>, Piotr A. Gauden<sup>2</sup>, Sylwester Furmaniak<sup>2</sup>, Artur P. Terzyk<sup>2</sup>, Marek Wiśniewski<sup>2</sup>, Jerzy Włoch<sup>3</sup> and Alexander V. Neimark<sup>4</sup>**

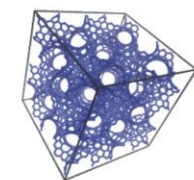
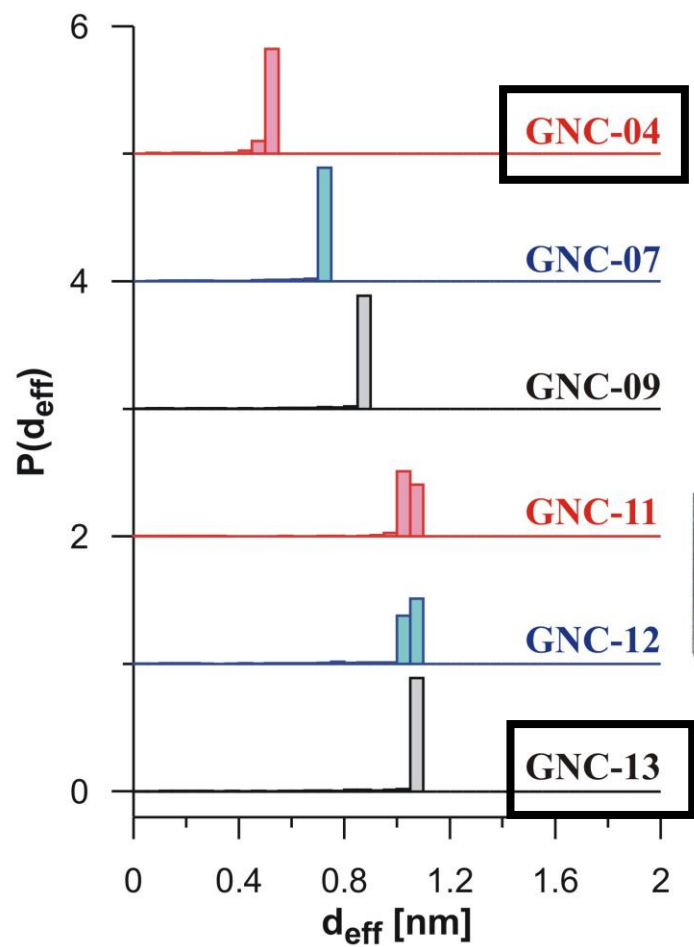
<sup>1</sup>School of Engineering and Information Technology, Murdoch University,  
Perth, Western Australia 6150

<sup>2</sup>Faculty of Chemistry, Physicochemistry of Carbon Materials Research Group,  
Nicolaus Copernicus University in Toruń, Gagarin Street 7, 87-100 Toruń,  
Poland

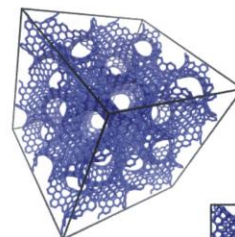
<sup>3</sup>Faculty of Chemistry, Synthesis and Modification of Carbon Materials  
Research Group, Nicolaus Copernicus University in Toruń, Gagarin Street 7,  
87-100 Toruń, Poland

<sup>4</sup>Department of Chemical and Biochemical Engineering, Rutgers, The State  
University of New Jersey, 98 Brett Road, Piscataway, New Jersey 08854-8058,  
United States

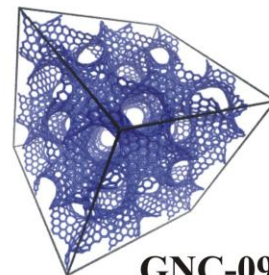




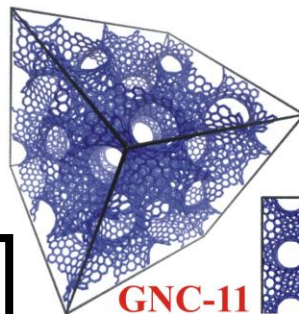
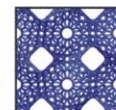
GNC-04



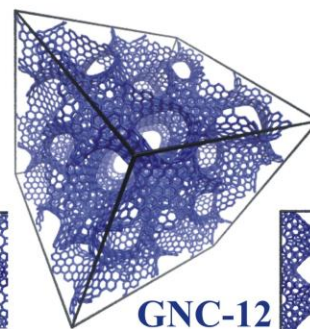
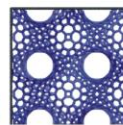
GNC-07



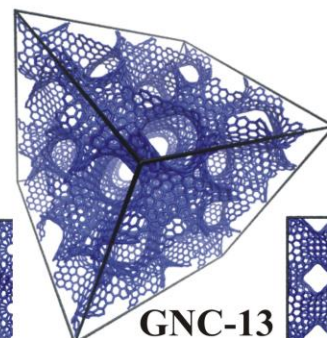
GNC-09



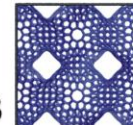
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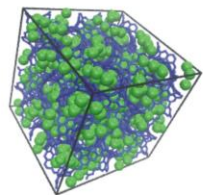
GNC-12



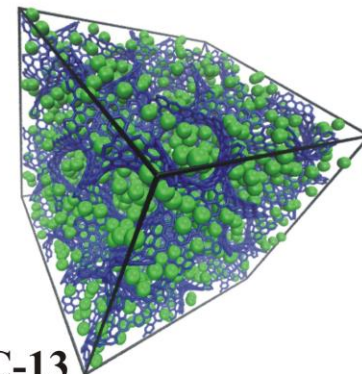
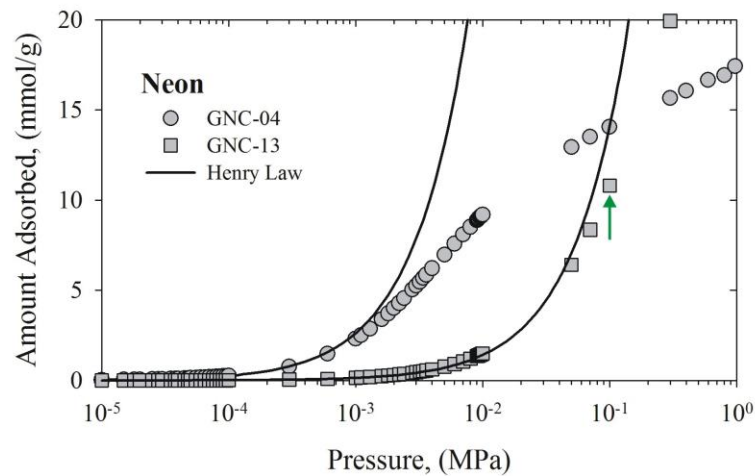
GNC-13



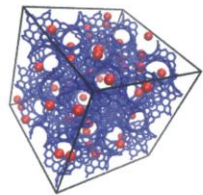
77 K



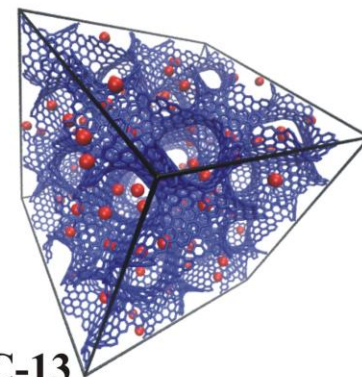
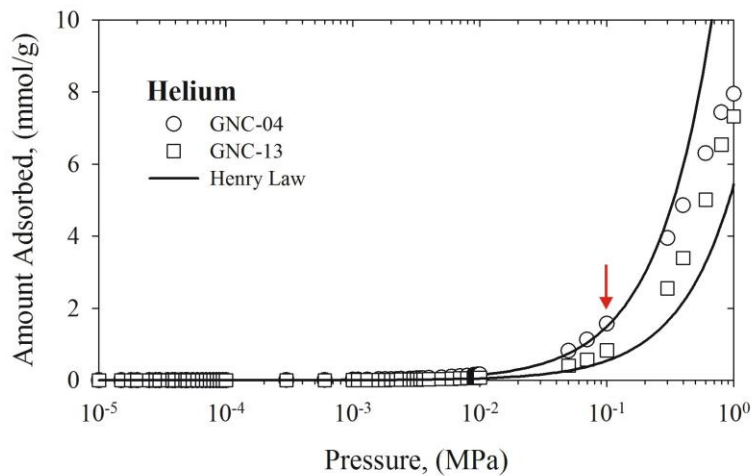
Ne: GNC-04



Ne: GNC-13

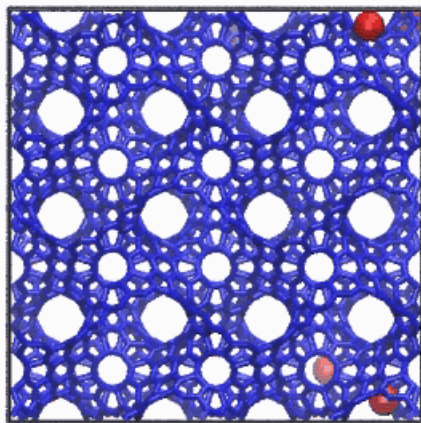


He: GNC-04

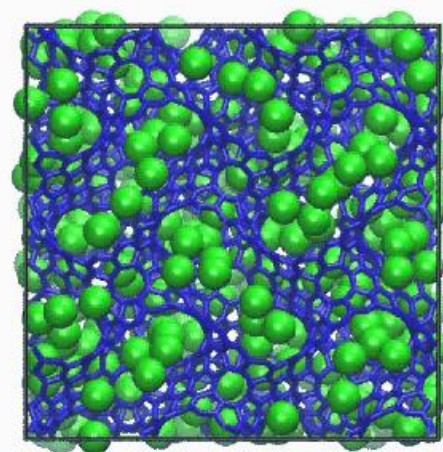


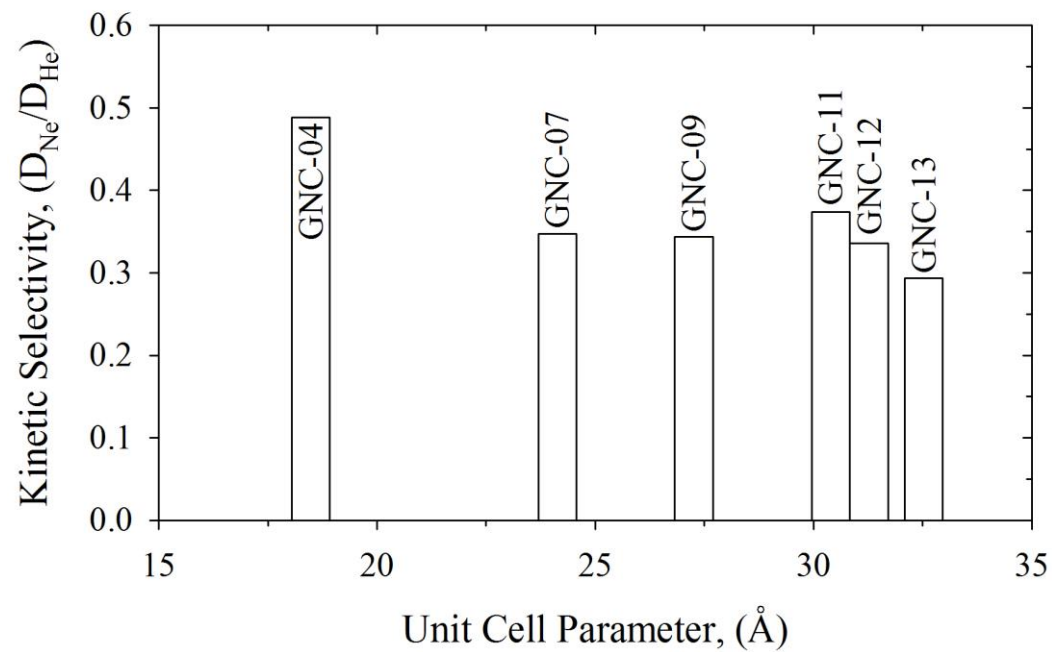
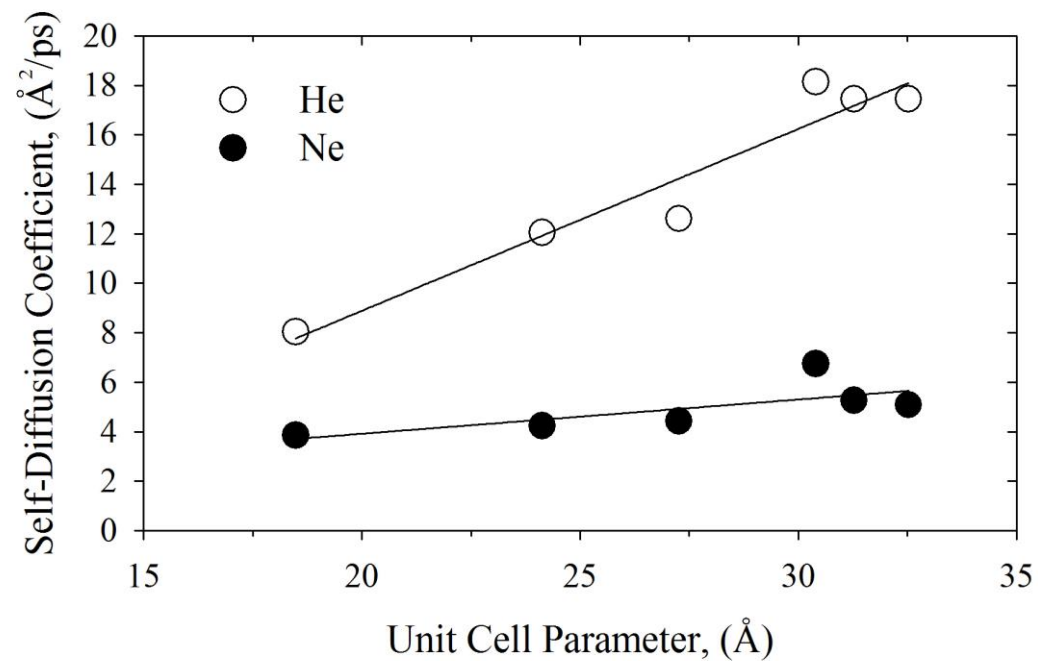
He: GNC-13

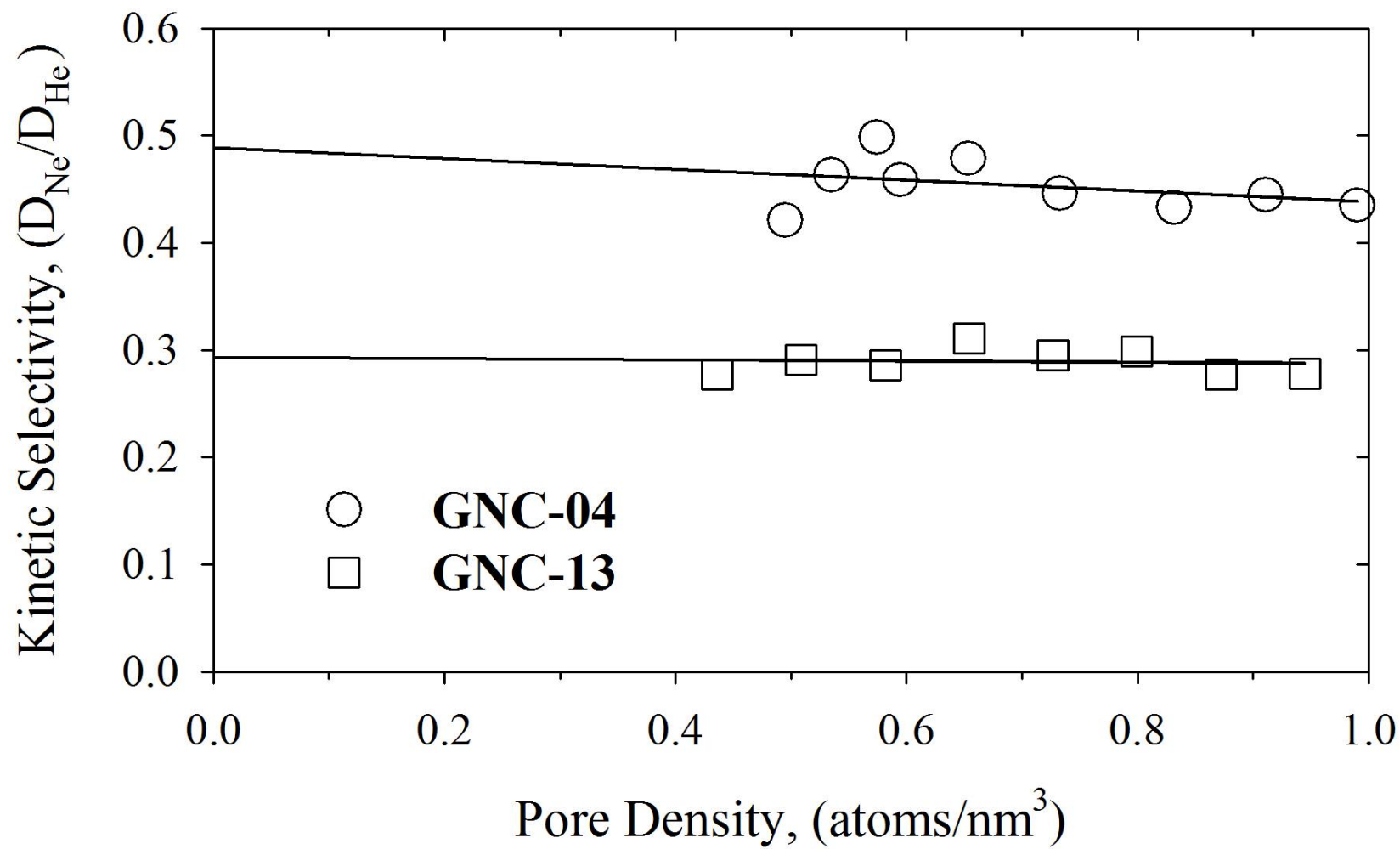
**He**  
**GNC-04**  
**T = 77 K**  
**p = 0.01 MPa**



**Ne**  
**GNC-04**  
**T = 77 K**  
**p = 0.01 MPa**



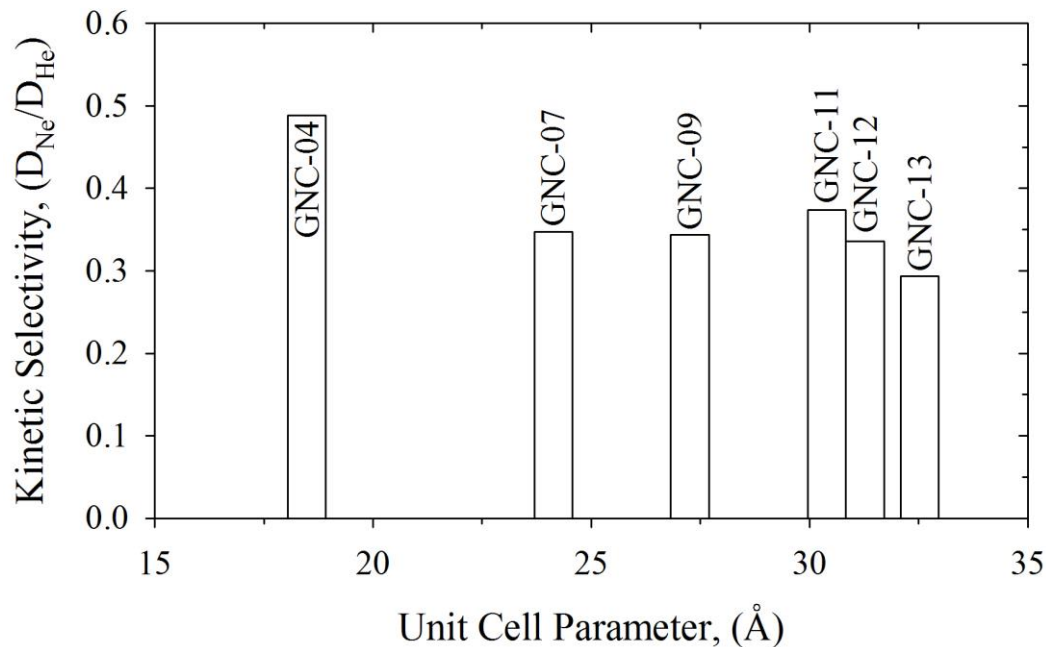
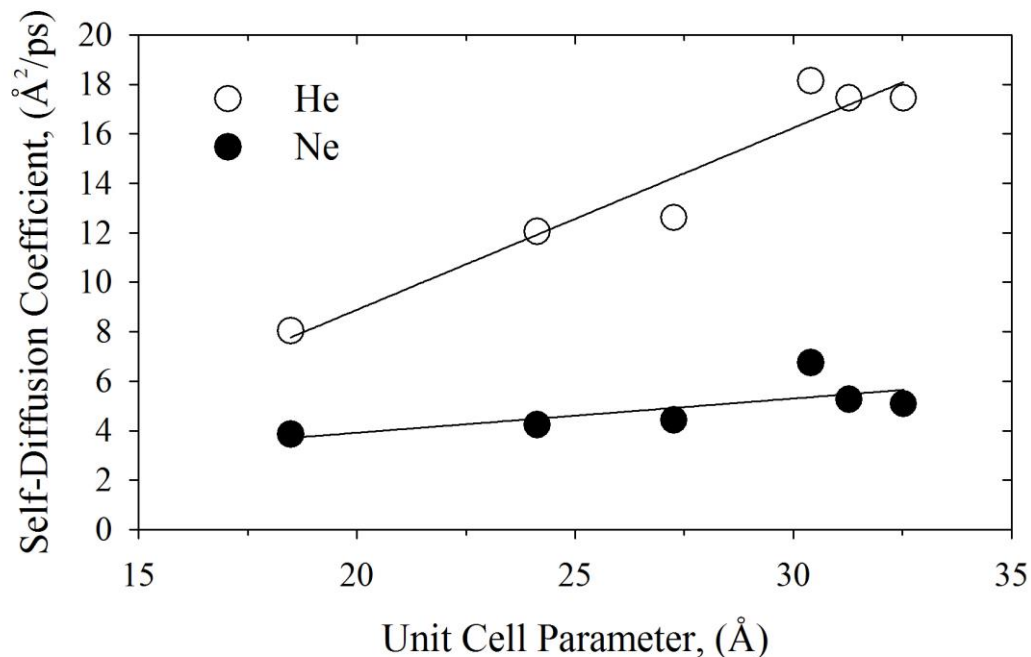




We find that selective separation of Ne from diluted Ne-He mixtures on microporous GNCs is driven by **preferential adsorption of Ne at 77 K**.

High adsorption-driven selectivity of Ne over He at zero coverage is compensated by an unfavourable Ne/He kinetic selectivity (e.g. faster diffusion of He).

A detailed analysis of theoretical and simulation results indicates that precise tuning of curved graphene ultramicropores in gyroidal carbon networks to  $\sim 0.53$  nm is a key for fabrication of selective carbon membranes for cryogenic separation technologies.

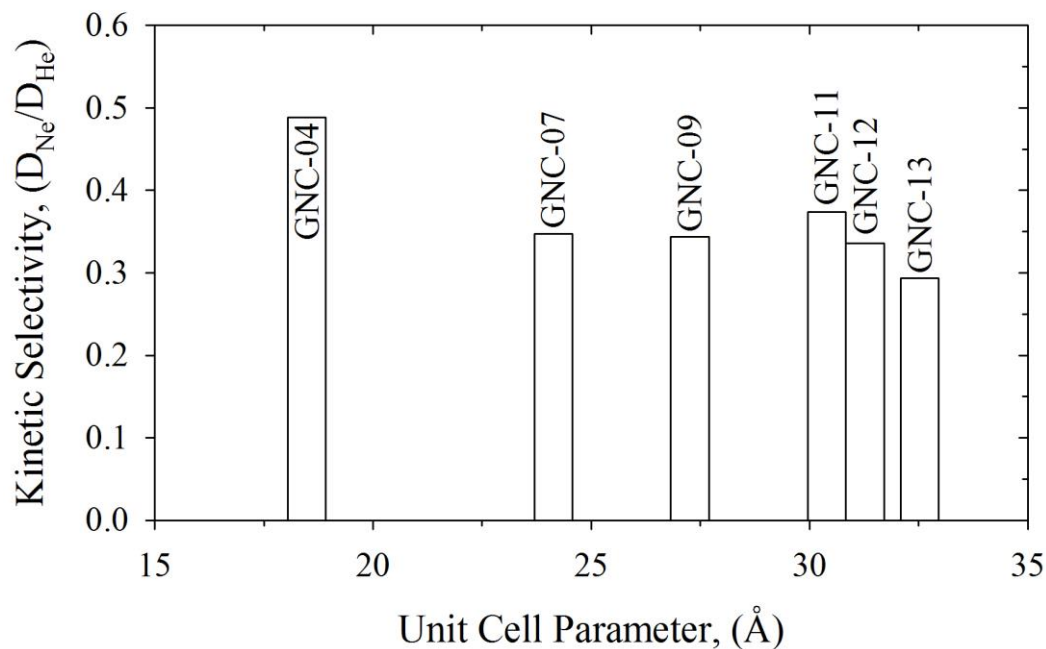
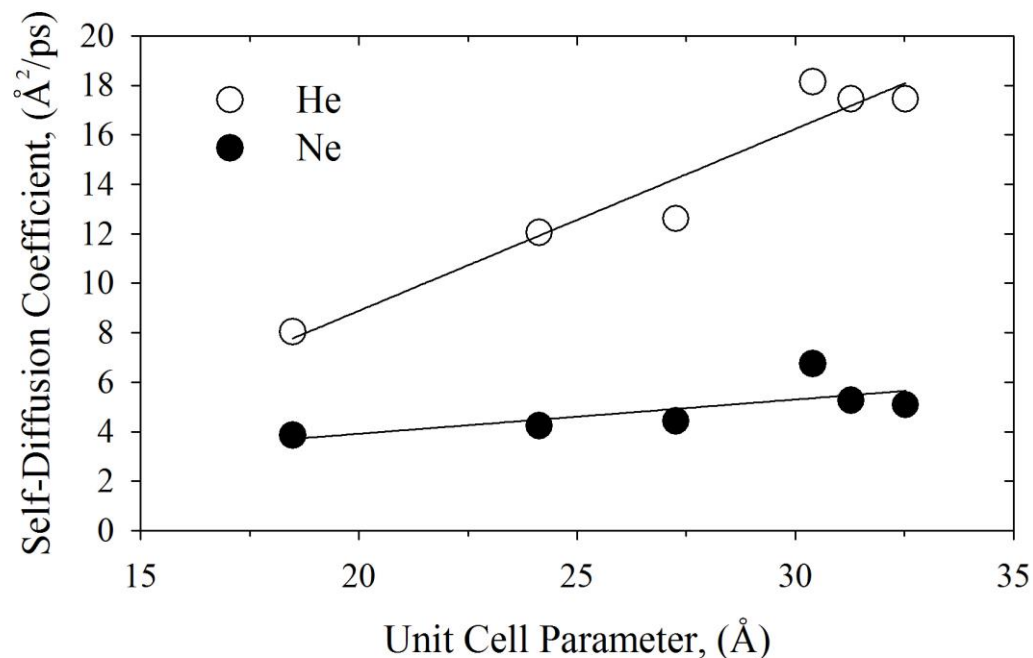




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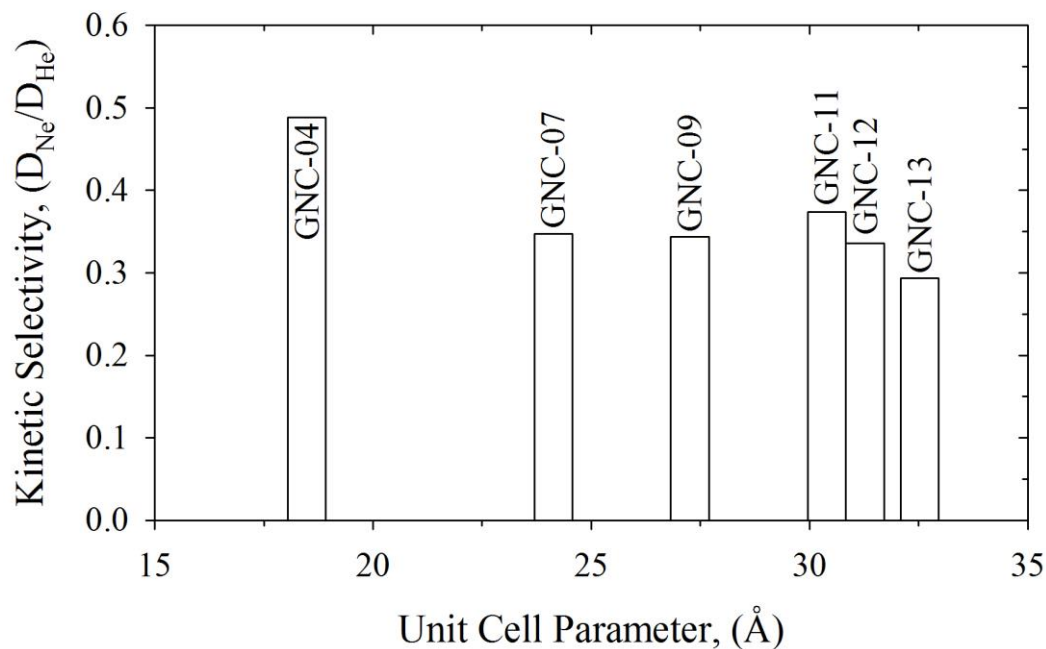
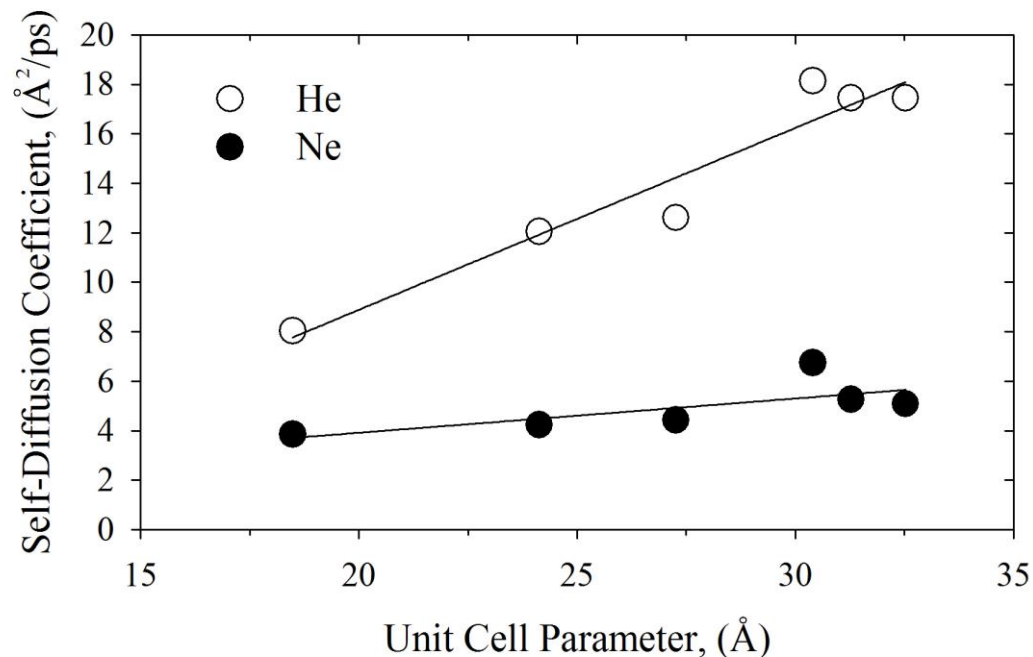




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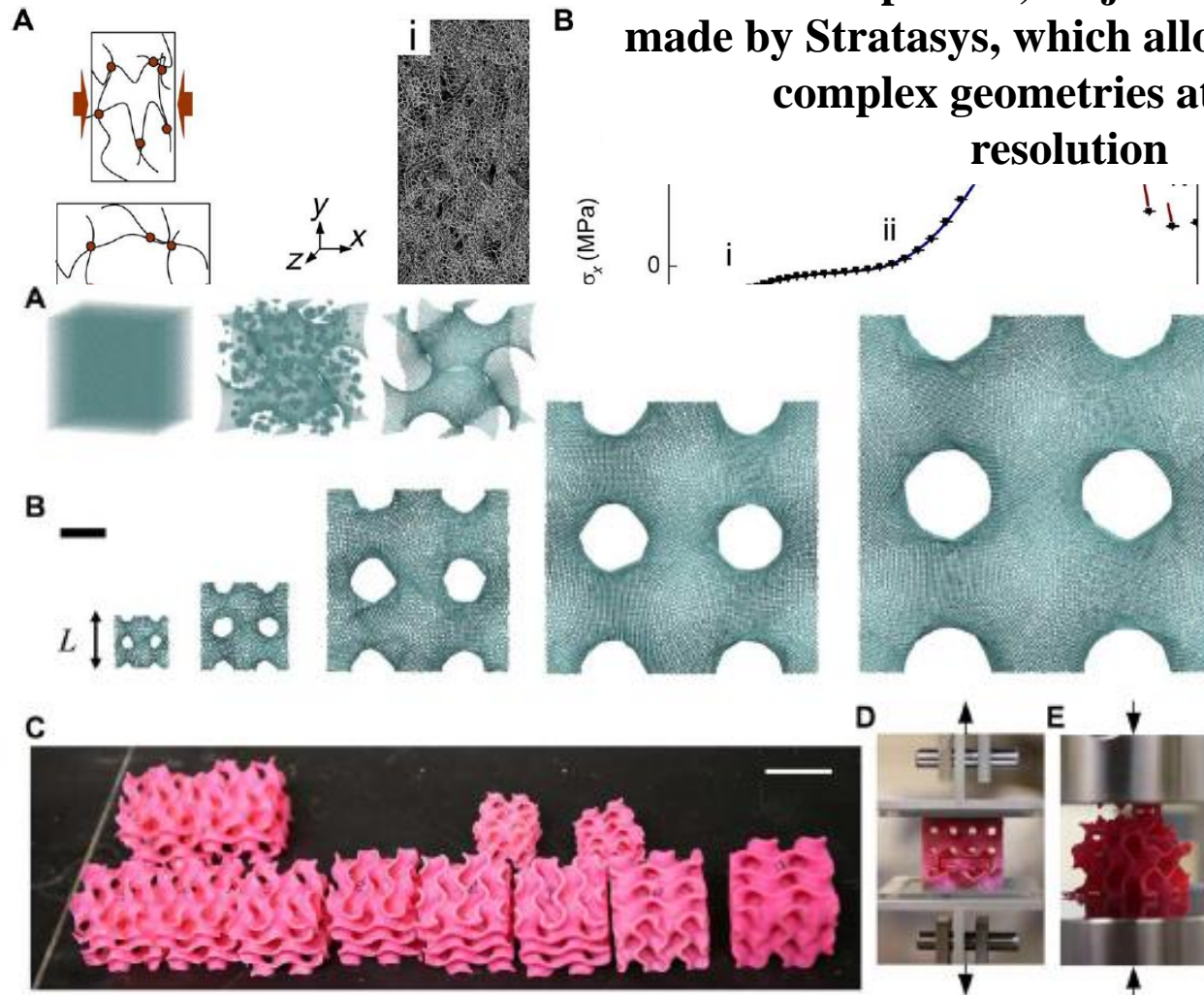
**MATERIALS SCIENCE**

# The mechanics and design of a lightweight three-dimensional graphene assembly

Zhao Qin,<sup>1\*</sup> Gang Seob Jung,<sup>1\*</sup> Min Jeong Kang,<sup>1</sup> Markus J. Buehler<sup>1,2†</sup>

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Commons Attribution  
4.0 International license.

made by Stratasys, which allowed us to print complex geometries at 20-mm resolution



**Fig. 4. Different atomistic and 3D-printed models of gyroid geometry for mechanical tests.** (A) Simulation snapshots taken during the modeling of the atomic 3D graphene structure with gyroid geometry, representing key procedures including (i) generating the coordinate of uniformly distributed carbon atoms based on the fcc structure, (ii) generating a gyroid structure with a triangular lattice feature, and (iii) refinement of the modified geometry from a gyroid with a triangular lattice to one with a hexagonal lattice. (B) Five models of gyroid graphene with different length constants of  $L = 3, 5, 10, 15$ , and  $20$  nm from left to right. Scale bar,  $25$  nm. (C) 3D printed samples of the gyroid structure of various  $L$  values and wall thicknesses. Scale bar,  $25$  cm. The tensile and compressive tests on the 3D printed sample are shown in (D) and (E), respectively.

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37 Rb Rubidium 84.468	38 Sr Strontium 87.62	39 Y Yttrium 88.906	40 Zr Zirconium 91.224	41 Nb Niobium 92.906	42 Mo Molybdenum 95.94	43 Tc Technetium 98.907	44 Ru Ruthenium 101.07	45 Rh Rhodium 102.906	46 Pd Palladium 106.42	47 Ag Silver 107.868	48 Cd Cadmium 112.411	49 In Indium 114.818	50 Sn Tin 118.71	51 Sb Antimony 121.760	52 Te Tellurium 127.6	53 I Iodine 126.904	54 Xe Xenon 131.29						
55 Cs Cesium 132.905	56 Ba Barium 137.327	57-71	72 Hf Hafnium 178.49	73 Ta Tantalum 180.948	74 W Tungsten 183.85	75 Re Rhenium 186.207	76 Os Osmium 190.23	77 Ir Iridium 192.22	78 Pt Platinum 195.08	79 Au Gold 196.967	80 Hg Mercury 200.59	81 Tl Thallium 204.383	82 Pb Lead 207.2	83 Bi Bismuth 208.980	84 Po Polonium [208.982]	85 At Astatine 209.987	86 Rn Radon 222.018						
87 Fr Francium 223.020	88 Ra Radium 226.025	89-103	104 Rf Rutherfordium [261]	105 Db Dubnium [262]	106 Sg Seaborgium [266]	107 Bh Bohrium [264]	108 Hs Hassium [269]	109 Mt Meitnerium [268]	110 Ds Darmstadtium [269]	111 Rg Roentgenium [272]	112 Cn Copernicium [277]	113 Uut Ununtrium unknown	114 Fl Flerovium [289]	115 Uup Ununpentium unknown	116 Lv Livermorium [293]	117 Uus Ununseptium unknown	118 Uuo Ununoctium unknown						

Lanthanide Series

57 <b>La</b> Lanthanum 138.906	58 <b>Ce</b> Cerium 140.115	59 <b>Pr</b> Praseodymium 140.908	60 <b>Nd</b> Neodymium 144.24	61 <b>Pm</b> Promethium 144.913	62 <b>Sm</b> Samarium 150.36	63 <b>Eu</b> Europium 151.966	64 <b>Gd</b> Gadolinium 157.25	65 <b>Tb</b> Terbium 158.925	66 <b>Dy</b> Dysprosium 162.50	67 <b>Ho</b> Holmium 164.930	68 <b>Er</b> Erbium 167.26	69 <b>Tm</b> Thulium 168.934	70 <b>Yb</b> Ytterbium 173.04	71 <b>Lu</b> Lutetium 174.967
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Actinide Series

89 <b>Ac</b> Actinium 227.028	90 <b>Th</b> Thorium 232.038	91 <b>Pa</b> Protactinium 231.036	92 <b>U</b> Uranium 238.029	93 <b>Np</b> Neptunium 237.048	94 <b>Pu</b> Plutonium 244.064	95 <b>Am</b> Americium 243.061	96 <b>Cm</b> Curium 247.070	97 <b>Bk</b> Berkelium 247.070	98 <b>Cf</b> Californium 251.080	99 <b>Es</b> Einsteinium [254]	100 <b>Fm</b> Fermium 257.095	101 <b>Md</b> Mendelevium 258.1	102 <b>No</b> Nobelium 259.101	103 <b>Lr</b> Lawrencium [262]
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Alkali Metal	Alkaline Earth	Transition Metal	Semimetal	Nonmetal	Basic Metal	Halogen	Noble Gas	Lanthanide	Actinide
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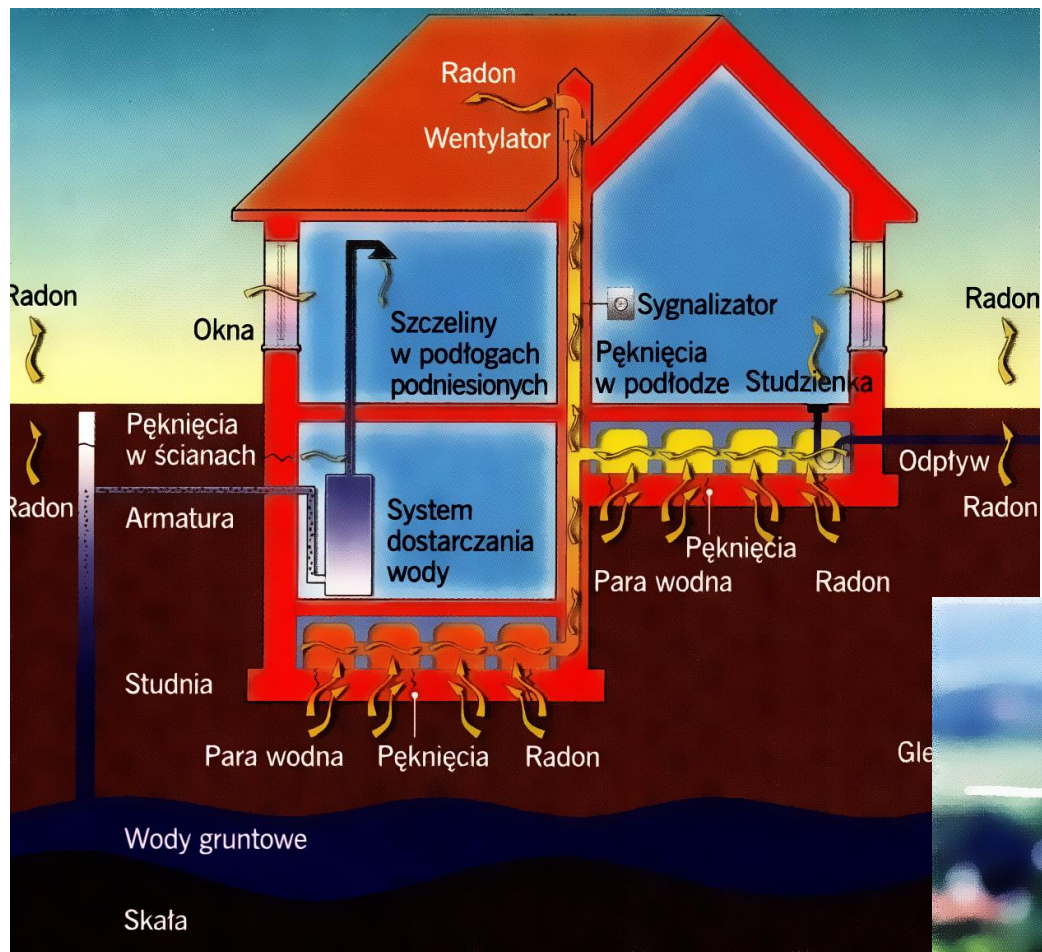
PUSTYNNY ZAMEK HERODA

# Prediction of Radon-222 Phase Behavior by Monte Carlo Simulation

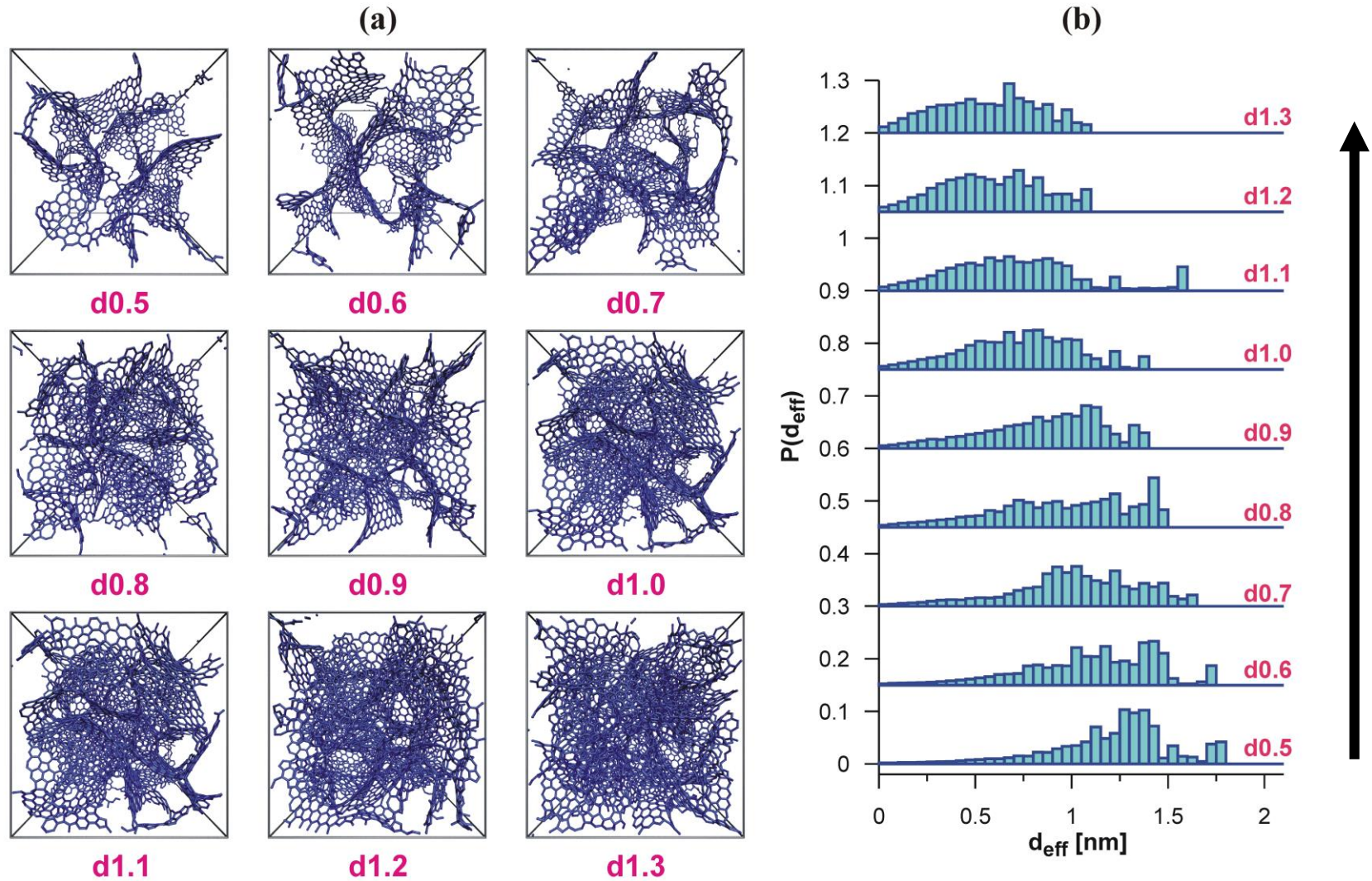
Jason R. Mick, Mohammad Soroush Barhaghi, and Jeffrey J. Potoff\*

*J. Chem. Eng. Data* 2016, 61, 1625–1631



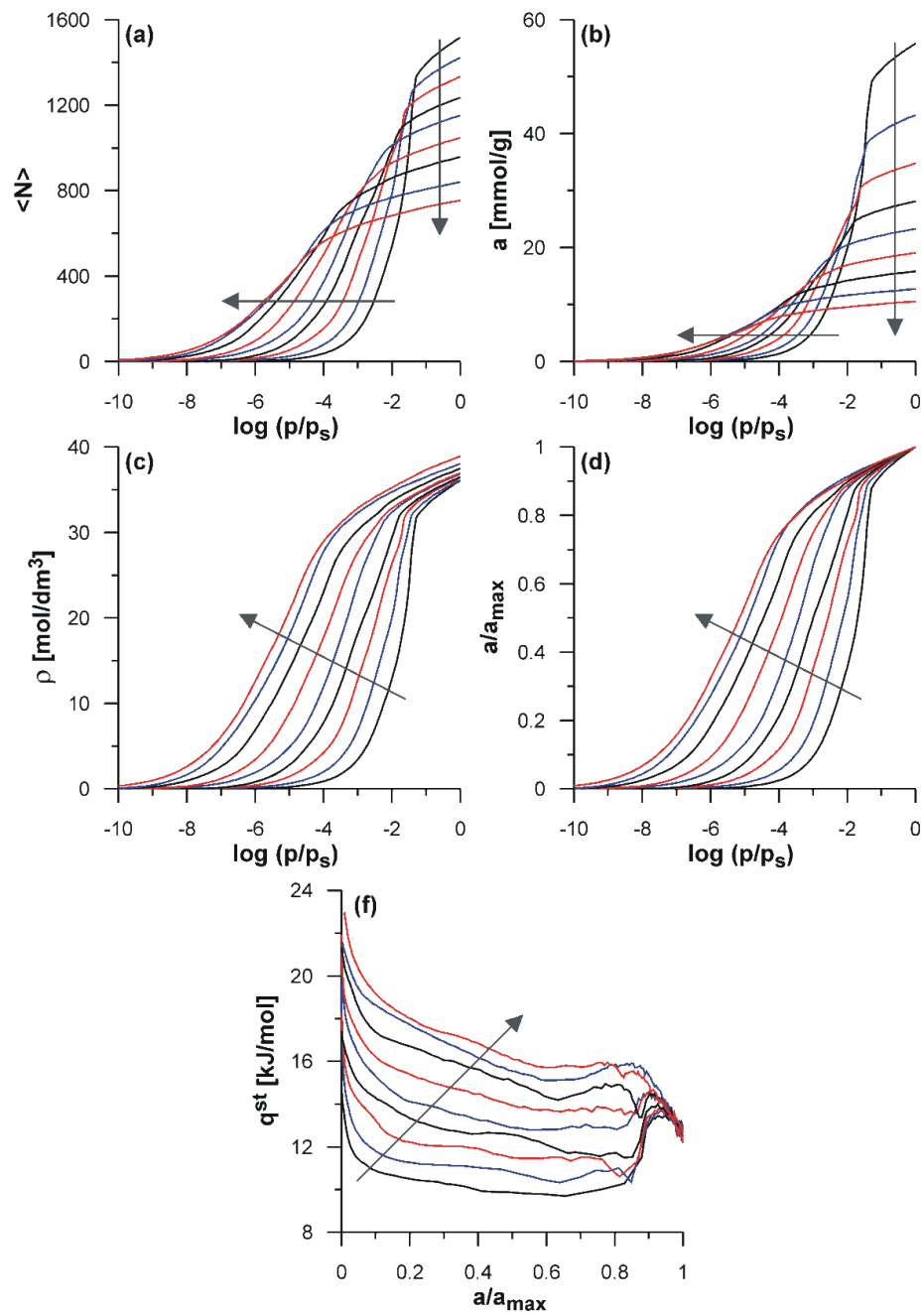


# Virtual Porous Carbons (VPCs)



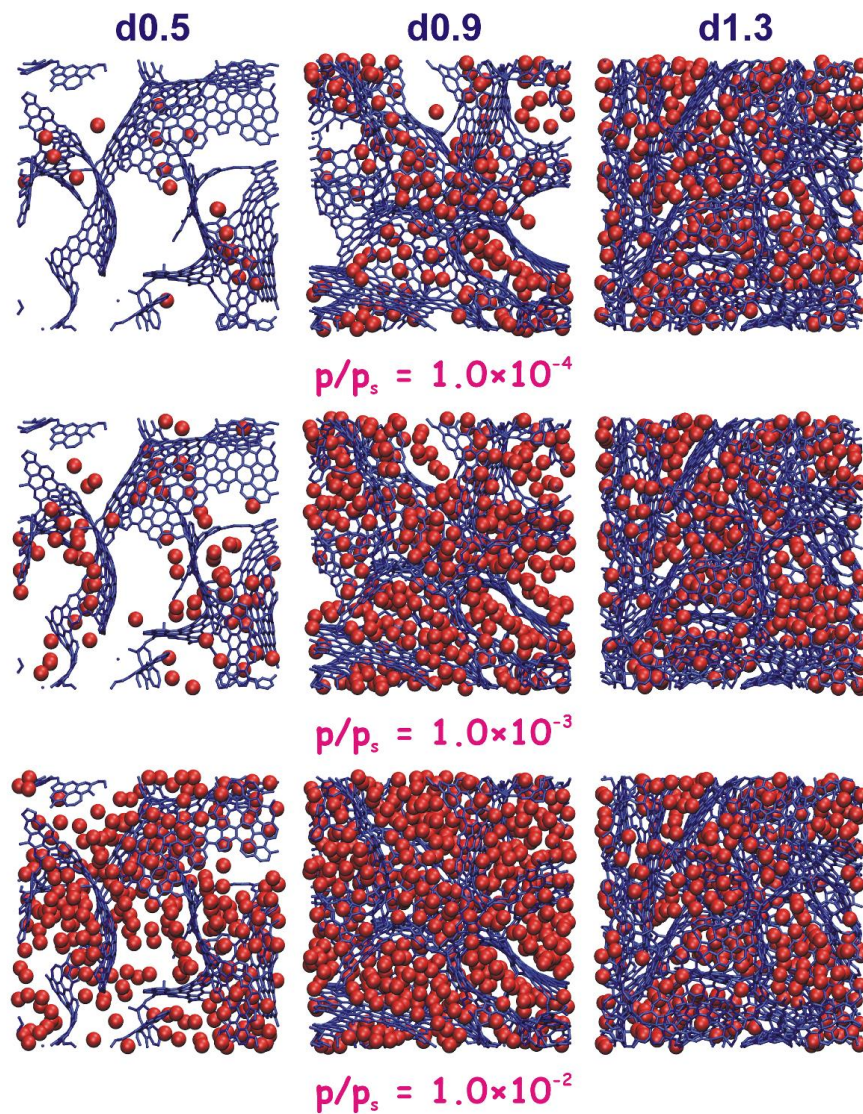
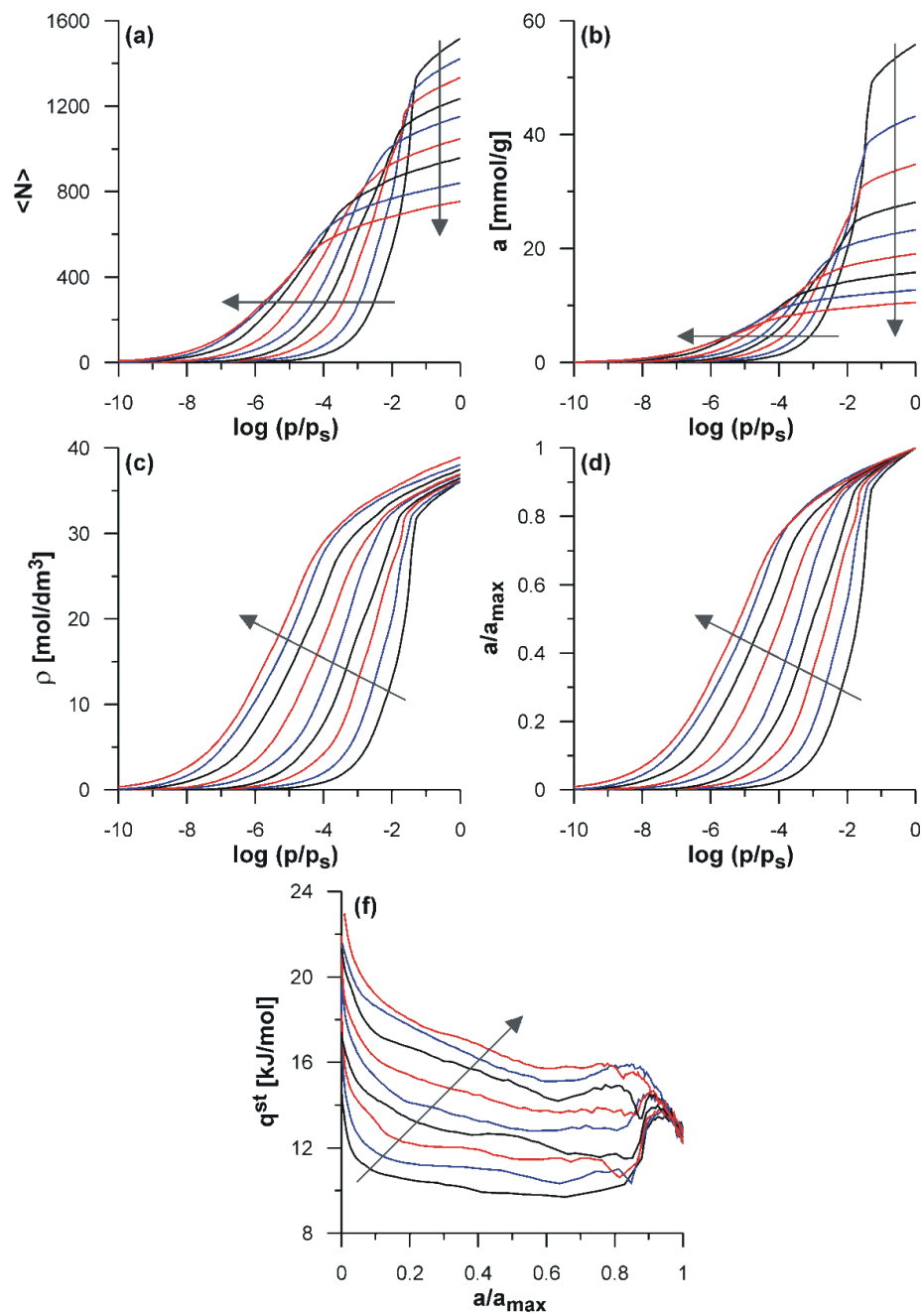
[S. Furmaniak, *Comput. Methods Sci. Technol.* 19 (2013) 47 ]

# Ar, 87 K

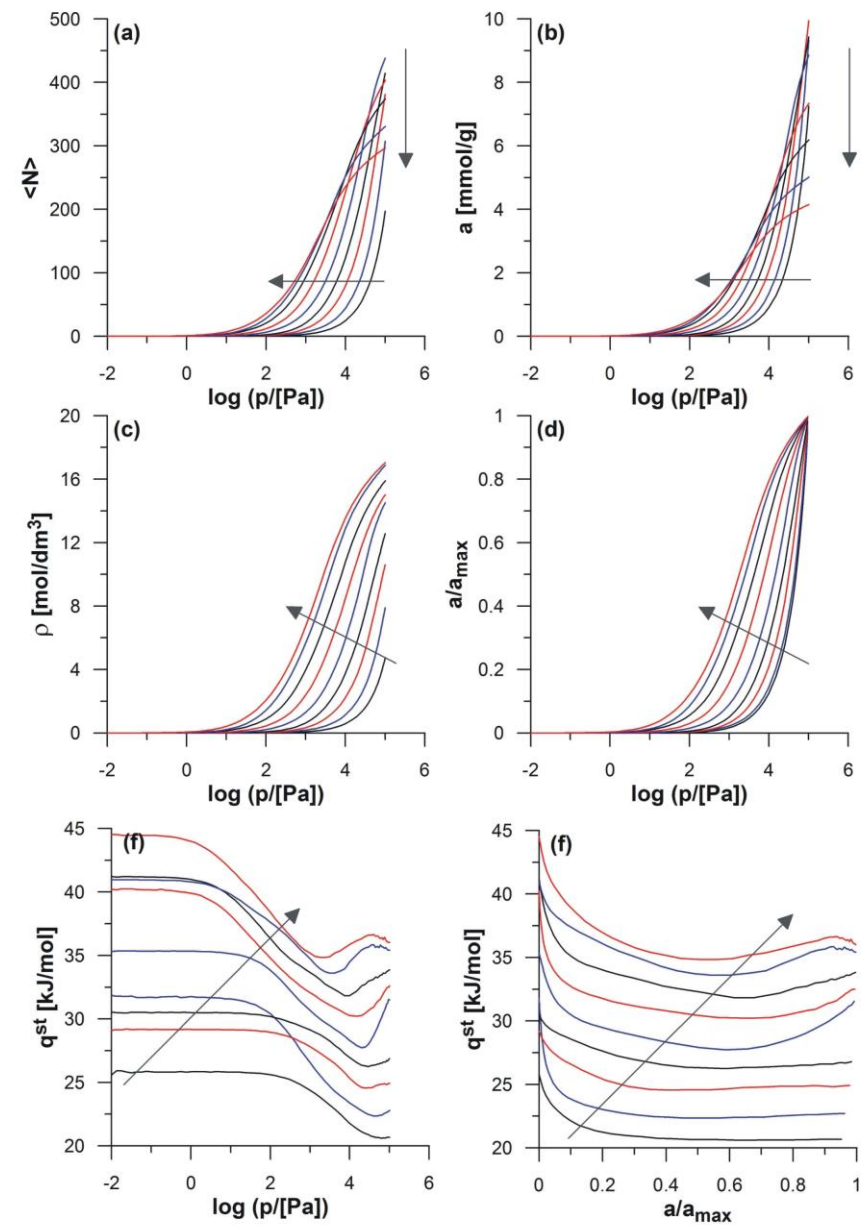




# Ar, 87 K

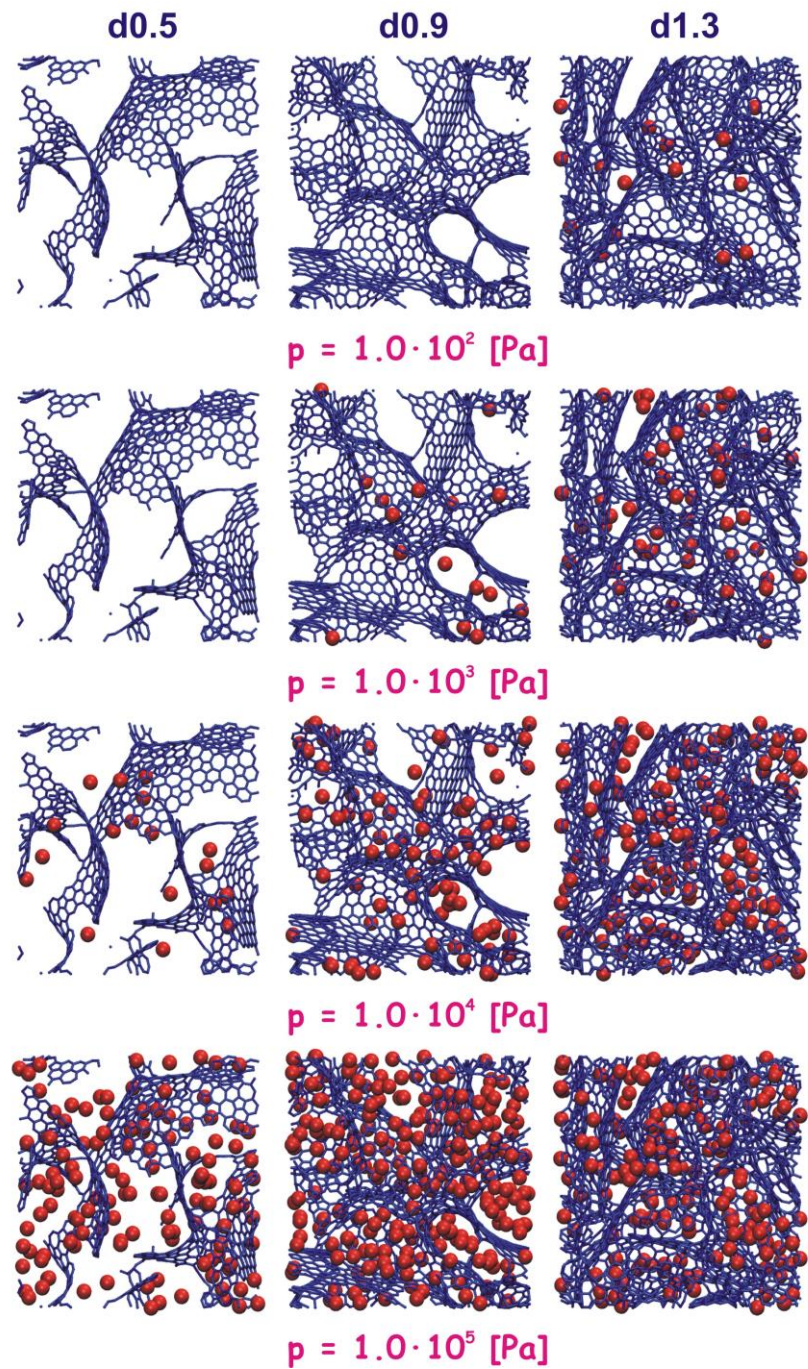
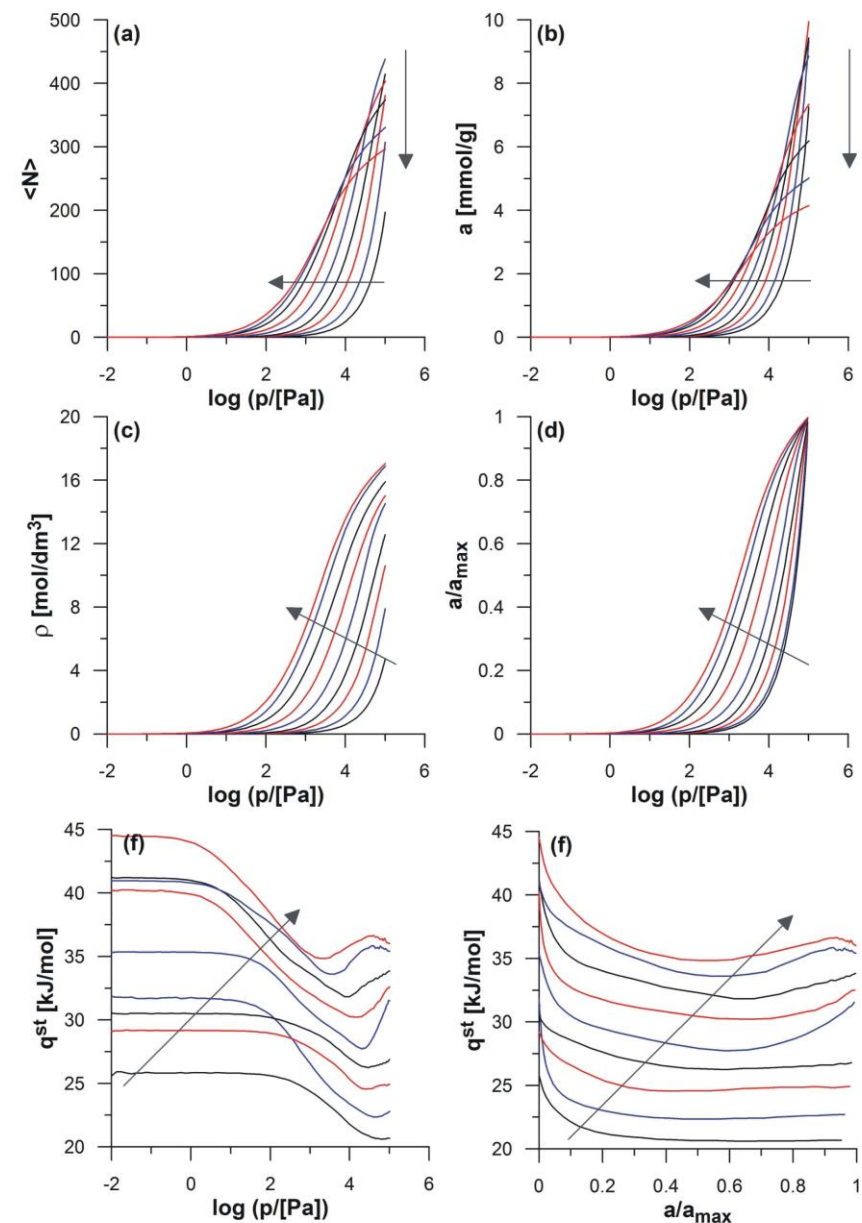


# Rn, 298 K





# Rn, 298 K





**Thank you**