INSTITUT LUMIÈRE MATIÈRE

topologie et géométrie des surfaces: une clef pour comprendre les structures de carbone

Patrice Mélinon,
[1]ILM and Université Lyon 1, Brillouin building,
campus Lyon Tech-La Doua, 69622
Villeurbanne France

cnrs
dépasser les frontières

Lyon 1

Materials (nano)science

Materials science includes those parts of chemistry, physics, geology and biology that deal with the physical, chemical or biological properties of materials.

Thermodynamics= thermostatic (optimized geometry)+ kinetics (metastable structures)
nobody knows the true ground state (example: carbon)

What is known in materials science (solid state physics) since one century!

All the properties (electronic, vibrational, magnetic,mechanical…) depend to the dimensionality (topological dimension)

d=-1 (vacuum, Casimir, Dirac…)

d=0 (clusters)

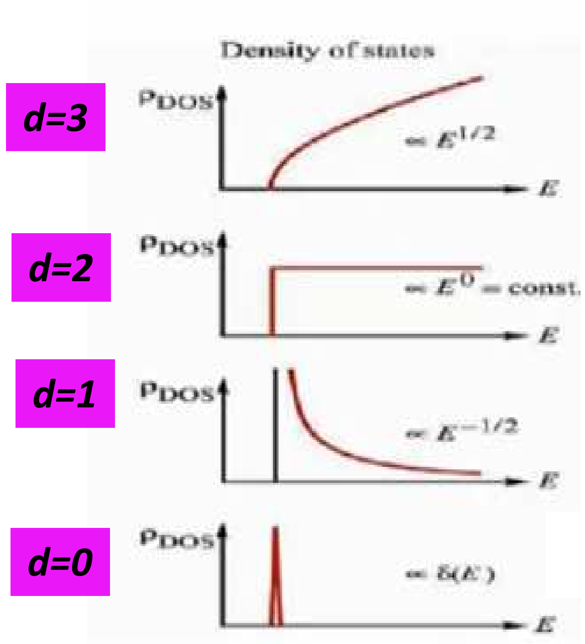
d=1 wire

d=2 (carbon, quantum well)

d=3 crystal

d not integer (fractal structure) Hausdorff dimension is not pertinent

d>3 (quasicrystals…)



The density of states is defined as the number of different states at a particular energy level that electrons are allowed to occupy

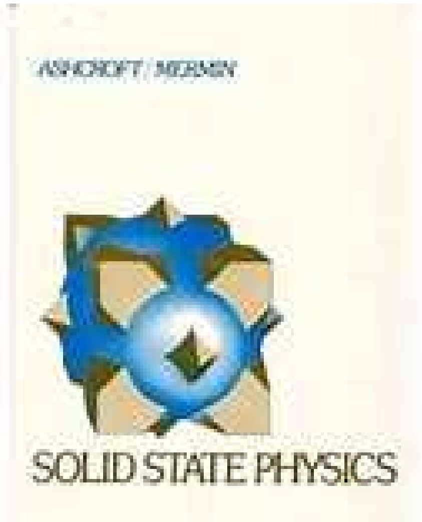
All the properties are (often) related to periodicity (cristallography)
Amorphous materials are a specific class
described as a « perturbed » crystal

In a semiconductor (insulator) few ppm of impurities
are enough to promote conduction!!!!

↓

electronic properties are sensitive to « environment »
(applications: electronic devices, sensors..)

The holly bible of the solid states physics
Ashcroft- Mermin book states



Cartesian product of three circles, $\mathbb{T}^3 = S^1 \times S^1 \times S^1$.

three-dimensional torus

chapter 2 page 33

but in 4D-space

" Thus if our metal is one dimensional we would simply replace the line from 0 to L to which the electron were confined by a circle of circumference L. In three dimensions the geometrical embodiment of the boundary condition , in which three pairs of opposite faces on the cube are joint , becomes topologically impossible to construct in three dimensional space "

Topology has invited itself in materials science

to date: connection between topology ang geometry using Gauss Bonnet theorem

geometry

intrinsic

extrinsic
differential, discrete

Macroscopic
« classical » physics

Microscopic (nano world)

topology

properties related to the topology

Evolution of the system
according to the topology rules
(homotopy)
Thermodynamics (kinetics pathways)

topology rules breakdown

phase transition

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Topology and geometry (hyperbolic for example) are emergent

Duncan Haldane, Micheal Kosterlitz et David Thouless

Nobel price 2016

Topological insulators

A topological insulator, like an ordinary insulator, has a bulk energy gap separating the highest occupied electronic band from the lowest empty band. The surface (or edge in two dimensions) of a topological insulator, however, necessarily has gapless states that are protected by time-reversal symmetry.

Scientific Research Publishing

Journal of Modern Physics, 2019, 10, 102-127
http://www.scirp.org/journal/jmp
ISSN Online: 2153-120X
ISSN Print: 2153-1196

A Topological Transformation of Quantum Dynamics

Vu B. Ho

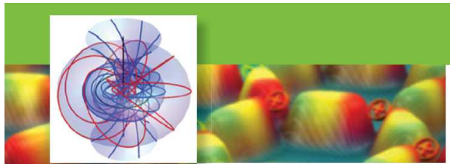
Advanced Study, 9 Adela Court, Mulgrave, Australia
Email: vubho@bigpond.net.au

Amazing properties

- *Insulator (bulk)*
- *Conducting (surface)*
- *Conduction is independent from the surface chemistry!!!!*

Topologically protected states (topological invariants, i.e. which don't depends of local physics as impurities or so on.

Topology and geometry (hyperbolic for example) are emergent




A topological twist on materials science

Sanju Gupta and Avadh Saxena

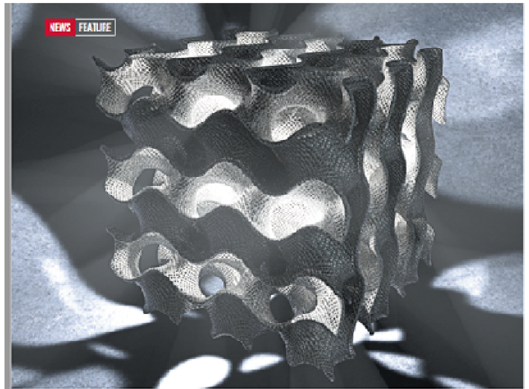
The primary objective of this article is twofold: to address the key concept of topology that impacts materials science in a major way and to convey the excitement to the materials community of recent significant advances in our understanding of the important topological notions in a wide class of materials with potential technological applications. A paradigm of topology/geometry → property → functionality is emerging that goes beyond the traditional microscopic structure → property → functionality relationship. The new approach delineates the active roles of topology and geometry in design, fabrication, characterization, and predictive modeling of novel materials properties and multifunctionalities. After introducing the essentials of topology and geometry, we elucidate these concepts through a gamut of nanocarbon allotropes of *de novo* carbons, hierarchical self-assembled soft- and biomaterials, supramolecular assemblies, and nanoporous materials. Applications of these topological materials range from sensing, energy storage/conversion, and catalysis to nanomedicine.

MRS BULLETIN • VOLUME 39 • MARCH 2014 • www.mrs.org/bulletin 265

Topological invariants of time-reversal-invariant band structures

J. E. Moore[1,2] and L. Balents[3]
[1]Department of Physics, University of California, Berkeley, CA 94720
[2]Materials Sciences Division, Lawrence Berkeley National Laboratory, Berkeley, CA 94720
[3]Department of Physics, University of California, Santa Barbara, CA 93106
(Dated: February 4, 2008)

The topological invariants of a time-reversal-invariant band structure in two dimensions are multiple copies of the $\mathbb{Z}_2$ invariant found by Kane and Mele. Such invariants protect the topological insulator and give rise to a spin Hall effect carried by edge states. Each pair of bands related by time reversal is described by a single $\mathbb{Z}_2$ invariant, up to one less than half the dimension of the Bloch Hamiltonians. In three dimensions, there are four such invariants per band. The $\mathbb{Z}_2$ invariants of a crystal determine the transitions between ordinary and topological insulators as its bands are occupied by electrons. We derive these invariants using maps from the Brillouin zone to the space of Bloch Hamiltonians and clarify the connections between $\mathbb{Z}_2$ invariants, the integer invariants that underlie the integer quantum Hall effect, and previous invariants of $\mathcal{T}$-invariant Fermi systems.



THE SHAPE OF THINGS TO COME

Strange topological effects might be hiding inside perfectly ordinary materials. Finding them could reveal new particles, deliver superfast transistors and even bolster quantum computing.

272 | NATURE | VOL 547 | 20 JULY 2017

carbon

→ *floppy element*

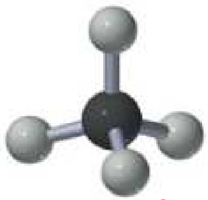
→ *most studied element*

→ *most useful (organic chemistry, living thing)*

→ *allotropes: diamond , fullerenes, onions, nanotubes, origamis, clathrate, graphite, amorphous carbon, liquid carbon…*

→ *remains a piece of mystery (vitreous carbon ?)*

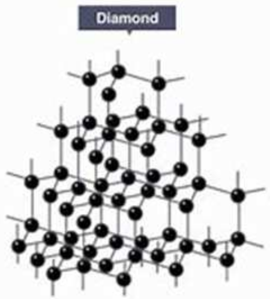
surfaces: one candidate (and no more!) the carbon



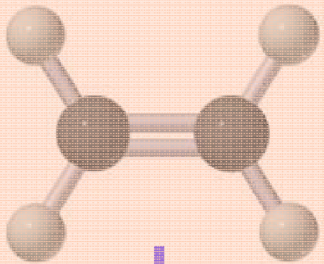
Carbon (sp^3 hybridization)

periodicity

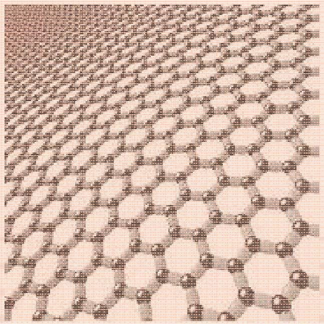
diamond (3Dstructure)



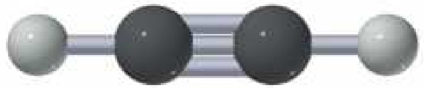
Carbon (sp^2 hybridization)



graphene (2D structure)



Carbon (sp hybridization)



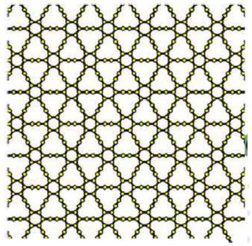
carbyne (1D structure)

carbon four electrons covalent bonding

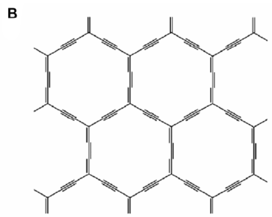
no periodicity

fullerene (0D structure) abusive!

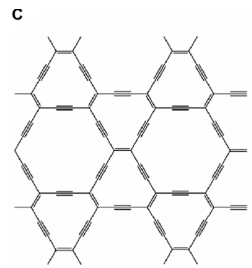
Peng et al https://doi.org/10.2147/NSA.S40324



γ-graphyne



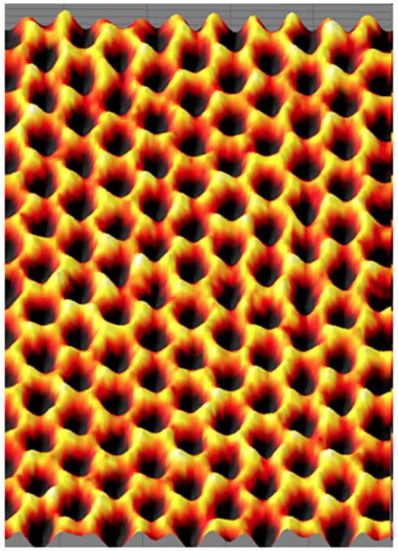
α-graphyne

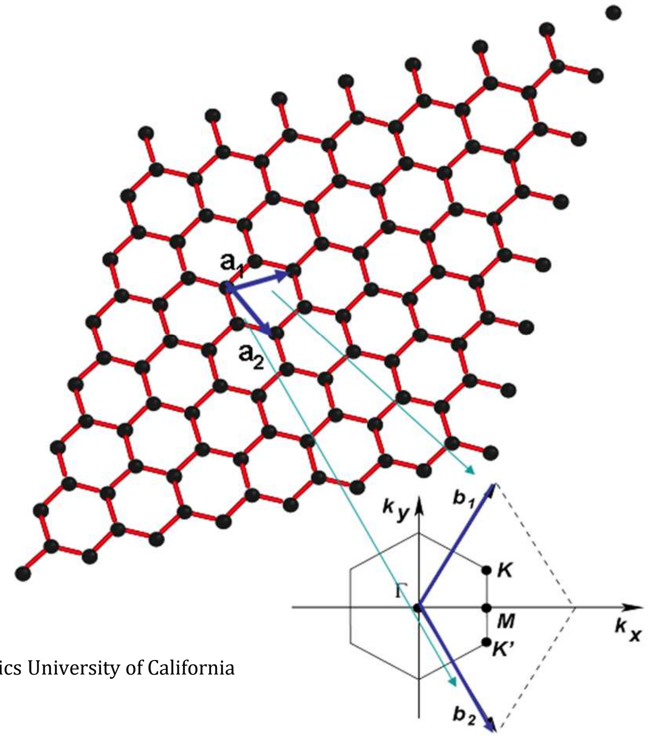


β-graphyne

Bieri, Marco, et al. Chemical communications 45 (2009): 6919-6921.

graphene

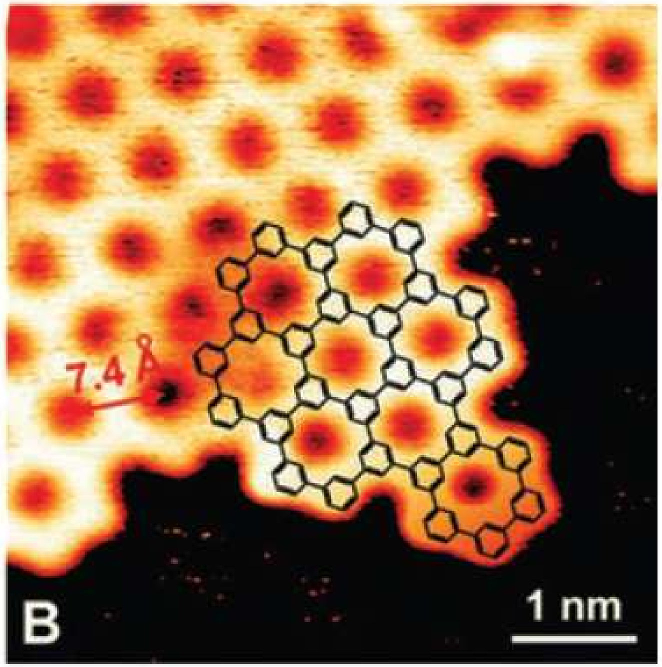




Zettl Research Group
Condensed Matter Physics Department of Physics University of California at Berkeley)

supergraphene

STM (Scanning Tunneling Microscope)



Graphene: topology opens the door

exceptionally high tensile strength, electrical conductivity, transparency

Electrons propagating through graphene's honeycomb lattice effectively lose their mass, producing quasi-particles that are described by a 2D analogue of the Dirac equation rather than the Schrödinger equation for spin-1/2 particles

2D Dirac-like Hamiltonian for massless fermions

classification theorem (surface)

PHYSICAL REVIEW B **102**, 115135 (2020)

Geometric approach to fragile topology beyond symmetry indicators

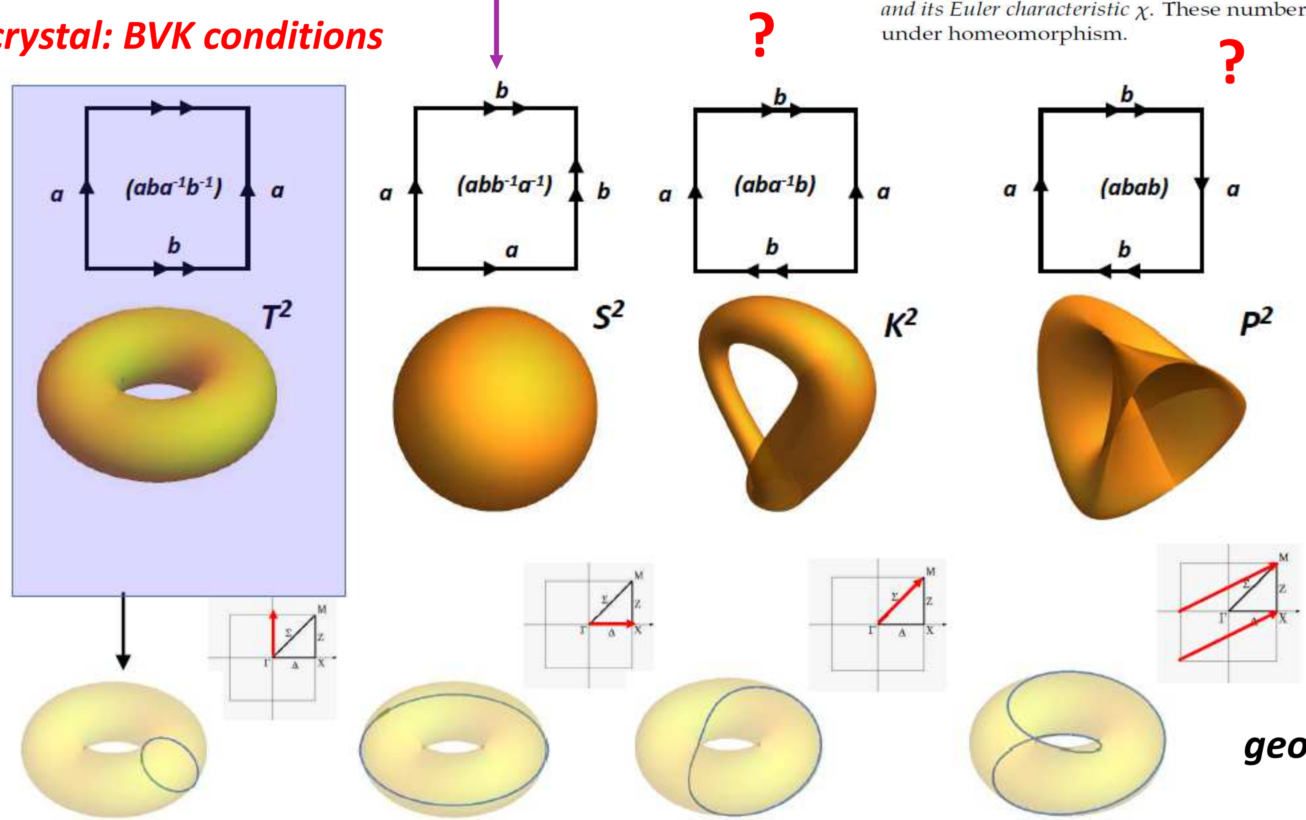
« strong » topological insulator

Theorem 1 ([61,62]). *Every compact (connected) surface is equivalent to one of the following three types of surfaces (see below for the definition):*

(i) *a sphere;*
(ii) *a connected sum of projective planes (if it is non-orientable); or*
(iii) *a connected sum of torii (if it is orientable and not a sphere).*

A compact surface is classified in terms of its boundary number β, its orientability number ω and its Euler characteristic χ. These numbers are topological invariants and are preserved under homeomorphism.

2D crystal: BVK conditions



geodesic

Toolbox for monitoring « symmetry »

Translational symmetry (crystal)

electron: fermion spin 1/2 *analogy with a fibre bundle*

but a toolbox is available

REVIEWS OF MODERN PHYSICS, VOLUME 82, OCTOBER–DECEMBER 2010

***Colloquium*: Topological insulators**

M. Z. Hasan[*]

Joseph Henry Laboratories, Department of Physics, Princeton University, Princeton, New Jersey 08544, USA

C. L. Kane[†]

Department of Physics and Astronomy, University of Pennsylvania, Philadelphia, Pennsylvania 19104, USA

(Published 8 November 2010)

Topological insulators are electronic materials that have a bulk band gap like an ordinary insulator but have protected conducting states on their edge or surface. These states are possible due to the combination of spin-orbit interactions and time-reversal symmetry. The two-dimensional (2D) topological insulator is a quantum spin Hall insulator, which is a close cousin of the integer quantum Hall state. A three-dimensional (3D) topological insulator supports novel spin-polarized 2D Dirac fermions on its surface. In this Colloquium the theoretical foundation for topological insulators and superconductors is reviewed and recent experiments are described in which the signatures of topological insulators have been observed. Transport experiments on HgTe/CdTe quantum wells are described that demonstrate the existence of the edge states predicted for the quantum spin Hall insulator. Experiments on $Bi_{1-x}Sb_x$, Bi_2Se_3, Bi_2Te_3, and Sb_2Te_3 are then discussed that establish these materials as 3D topological insulators and directly probe the topology of their surface states. Exotic states are described that can occur at the surface of a 3D topological insulator due to an induced energy gap. A magnetic gap leads to a novel quantum Hall state that gives rise to a topological magnetoelectric effect. A superconducting energy gap leads to a state that supports Majorana fermions and may provide a new venue for realizing proposals for topological quantum computation. Prospects for observing these exotic states are also discussed, as well as other potential device applications of topological insulators.

DOI: 10.1103/RevModPhys.82.3045 PACS number(s): 73.20.−r, 73.43.−f, 85.75.−d, 74.90.+n

Time-reversal symmetry
(spin-orbit coupling, magnetic field, magnetic element…)

Inversion symmetry (different chemical species
NB, dichacogenides…)

Glide reflection symmetry

Screw symmetry…

Gluing square and hexagon

In elemental structures square is never observed!

In 3D only one element with a simple cubic structure (cf Clifford torus) is observed (polonium)

never observed (excepted complex structures)

observed (graphene)

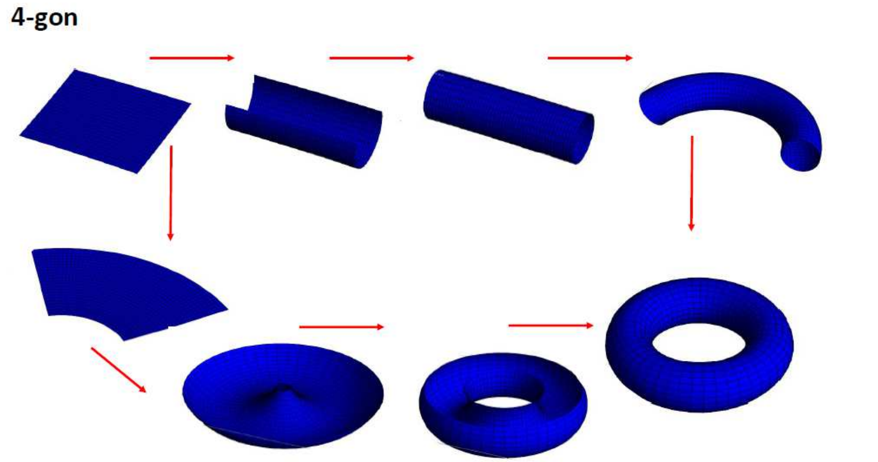
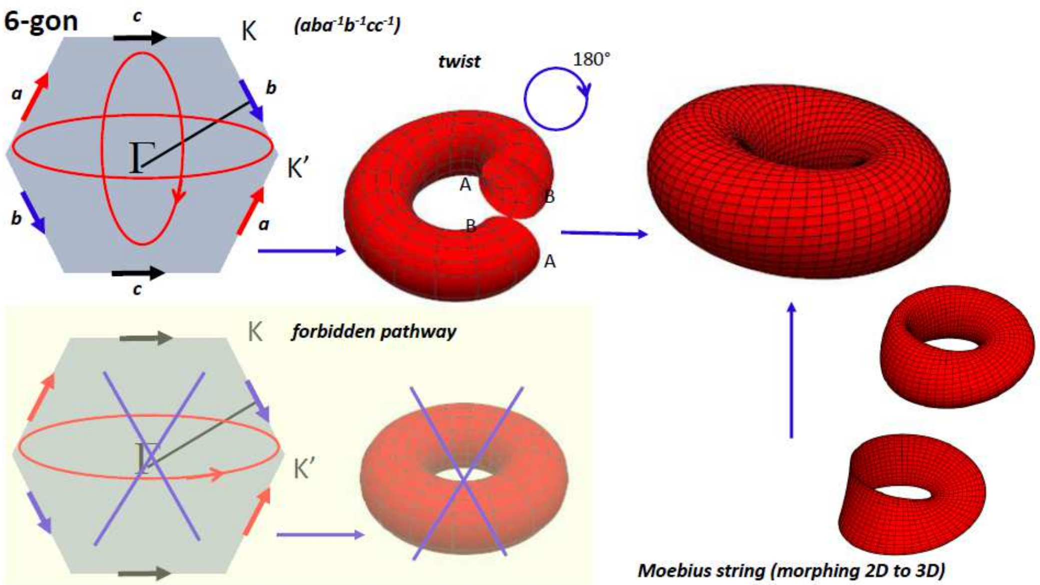
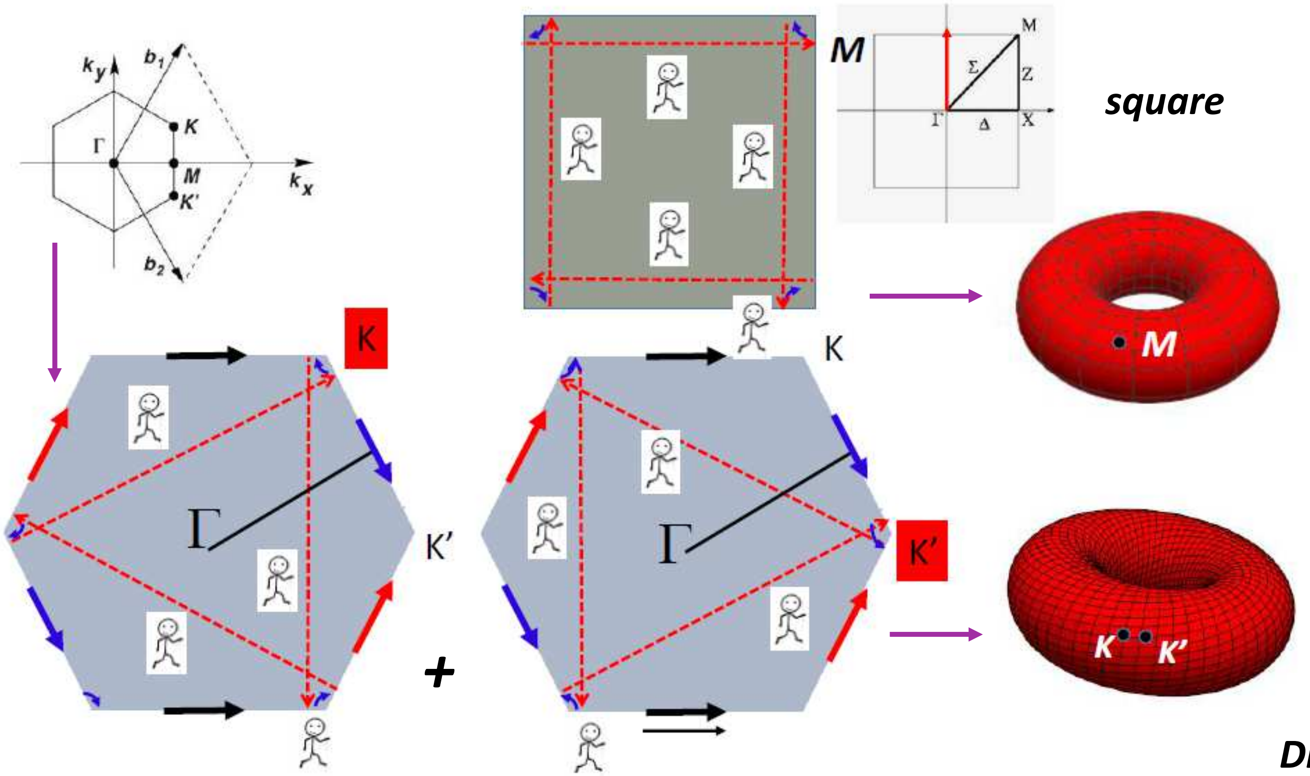


Figure 6. Two pathways for the flat torus formation corresponding to *BVK* conditions or Wallpaper group in crystallography.



Gluing hexagon

Graphene: amazing properties (Dirac cone entangled states with « massless » electrons)



electron mass m_e versus $-m_e$

« massless »

K,K' pair

Diract points (Pauli matrix)

topology

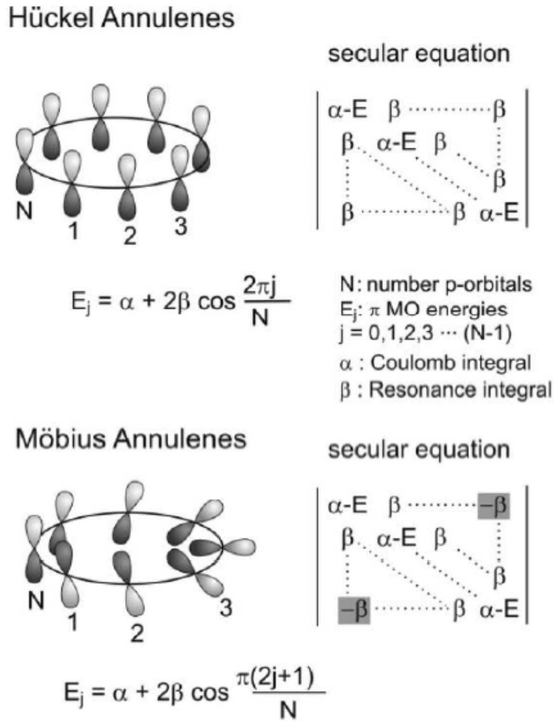
Properties are « different »   Example: topological insulators (torus to sphere)

States topologically protected
No modification under external perturbation
Impurities, defects…

Antiaromaticy (Moebius)

Thermodynamics (kinetics) according to homotopy rules
(self intersecting is forbidden for materials !)

Herges, R. Topology in chemistry: Designing Möbius molecules. *Chem. Rev.* **2006**, *106*, 4820–4842.



Hückel:	Möbius
4n+2 aromatic	4n aromatic
4n antiaromatic	4n+2 antiaromatic

Graphene and beyond : geometry opens the door

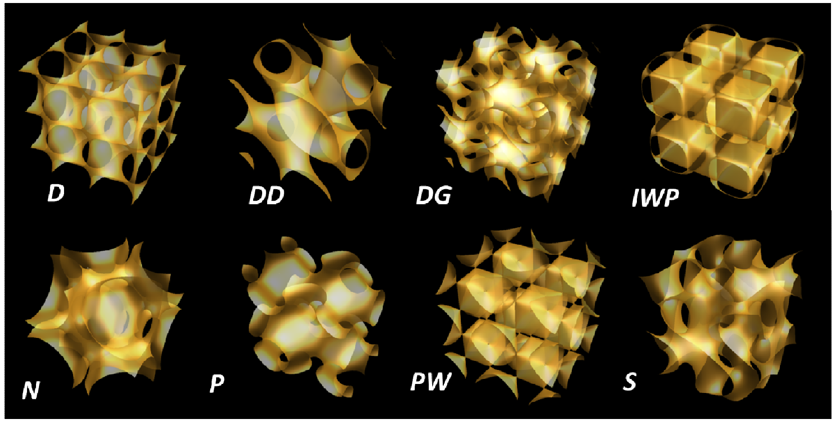
→ *hyperbolic geometry is poorly investigated by physicists*

Hyperbolic spaces: some examples in physics

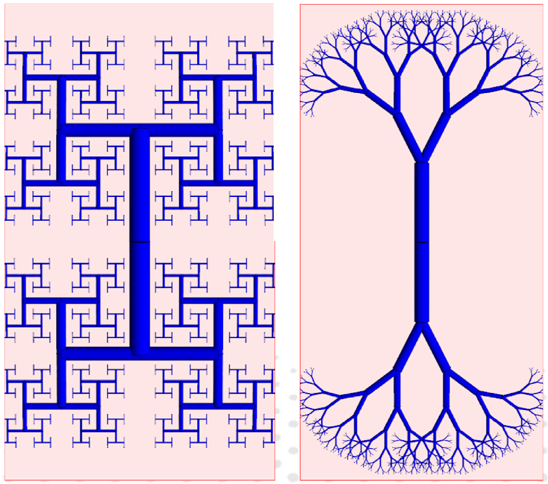
Physical phenomena are governed by the Laplacian

If Laplacian is « negative » chaos is possible (Hadamard)

opens the door of unusual properties (« fuite de Poincaré«, chaos…)



« continuous » (macroscopic samples)
3D printing



Fractal structure (lithography)

Microscopic: vitreous carbon

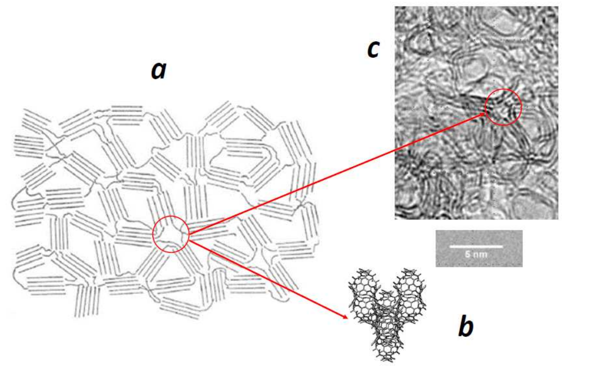


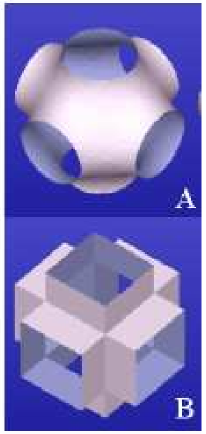
Figure 24. (**a**) Franklin's view of the *GLC*; (**b**) part of *HRTEM* pattern corresponding to the *GLC* produced by *PLD* and laser annealing (see Figure 5); and (**c**) an elemental cell of a Schwarzite *TPMS* structure [22].

Hyperbolic spaces: some examples in physics

Carbon: differential geometry
polymer printing+ pyrolysis
TPMS structures
Mechanical properties

Schwarz Meets Schwann: Design and Fabrication of Biomorphic Tissue Engineering Scaffolds

Srinivasan Rajagopalan and Richard A. Robb



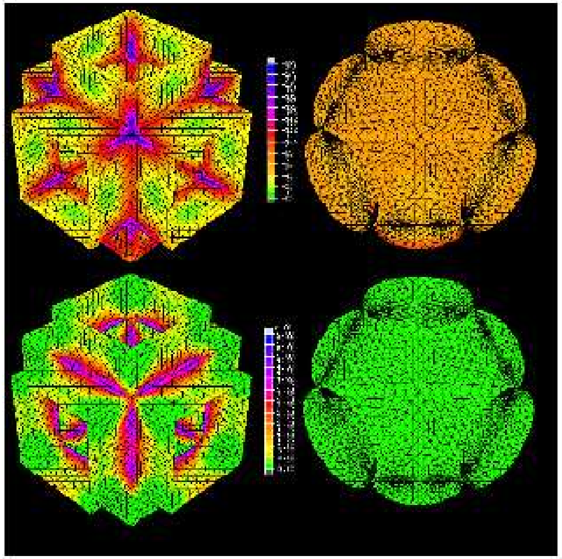


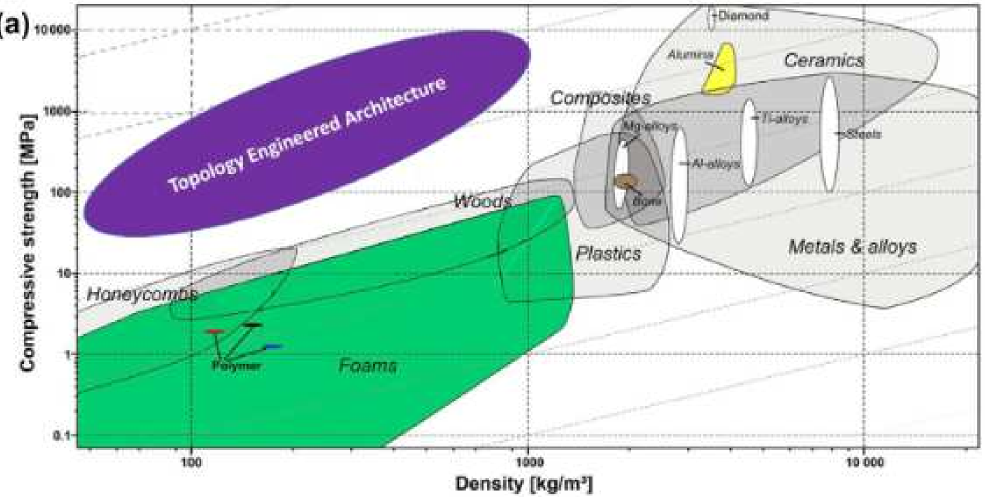
Fig. 7. Von Mises stress (top) and Principal Strain (bottom) maps under bulk compression for Cubic (left) and TPMS (right) unit cells (scale factor 1.0) with identical loading conditions and material properties

Materials Today • Volume 48 • September 2021 RESEARCH
ELSEVIER
RESEARCH: Review

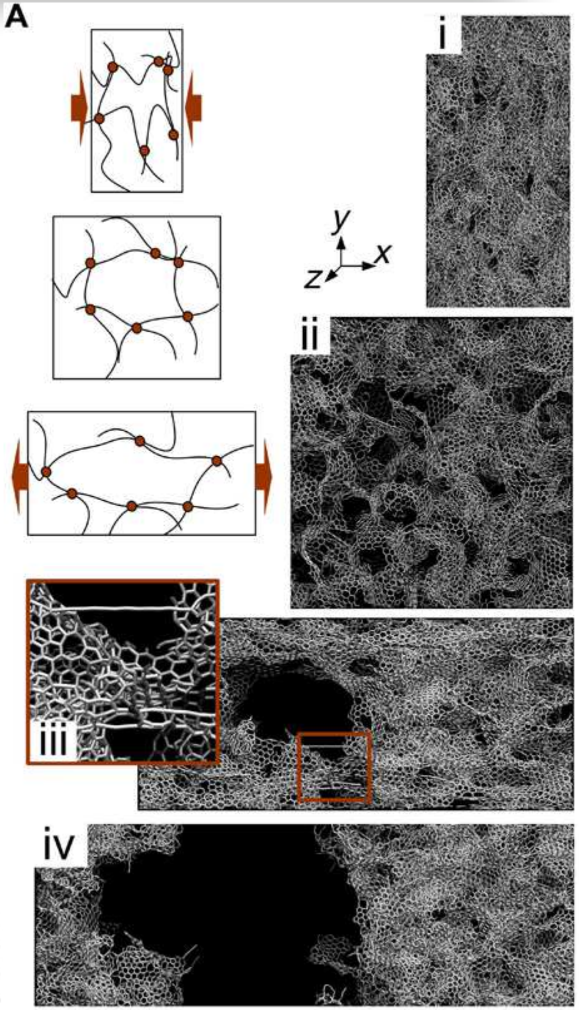
Topologically engineered 3D printed architectures with superior mechanical strength

Rushikesh S. Ambekar [1,†], Brijesh Kushwaha [1,†], Pradeep Sharma [2], Federico Bosia [3], Massimiliano Fraldi [4], Nicola M. Pugno [5,6,*], Chandra S. Tiwary [1,*]

(a)



TPMS carbon (macroscopic)



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

Zhao Qin[1,*], Gang Seob Jung[1,*], Min Jeong Kang[1] and Markus J. Buehler[1,2,†]
+ See all authors and affiliations

Science Advances 06 Jan 2017:
Vol. 3, no. 1, e1601536
DOI: 10.1126/sciadv.1601536

simulation/experiment
3D printing model

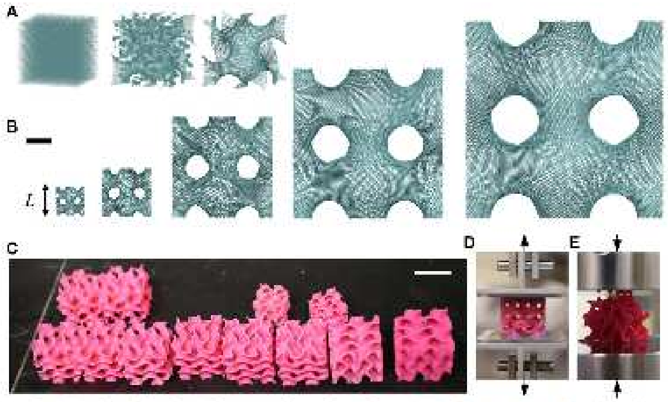


Fig. 4. Different atomistic and 3D-printed models of gyroid geometry for mechanical tests. (A) Simulation snapshots taken during the modeling of the atomic 3D graphene structure with gyroid geometry, representing key procedures including (i) generating the coordinate of uniformly distributed carbon atoms 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, 2.5 nm. (C) 3D-printed samples of the gyroid structure of various L values and wall thicknesses. Scale bar, 2.5 cm. The tensile and compressive tests on the 3D-printed sample are shown in (D) and (E), respectively.

sp^2 hybridization (six fold rings) mimics a true surface close to the mathematical concept

N=6 hexagons pure sp^2 hybridization (flat H=0 every where)

H (locally) ≠ 0 if homogeneous and isotrope depends to R the « radius »

Energetic point of view

N=5 pentagons « pure » sp^3 hybridization (pentagon 108° instead of 109,47° in fully sp^3 tetrahedron)

N=7 heptagons 128,57° not so far from 120°

N=4 90° corresponds to pure p bonding

N=8 heptagons 135° far from 120°

Euler's relationship (do not depend to N_6)

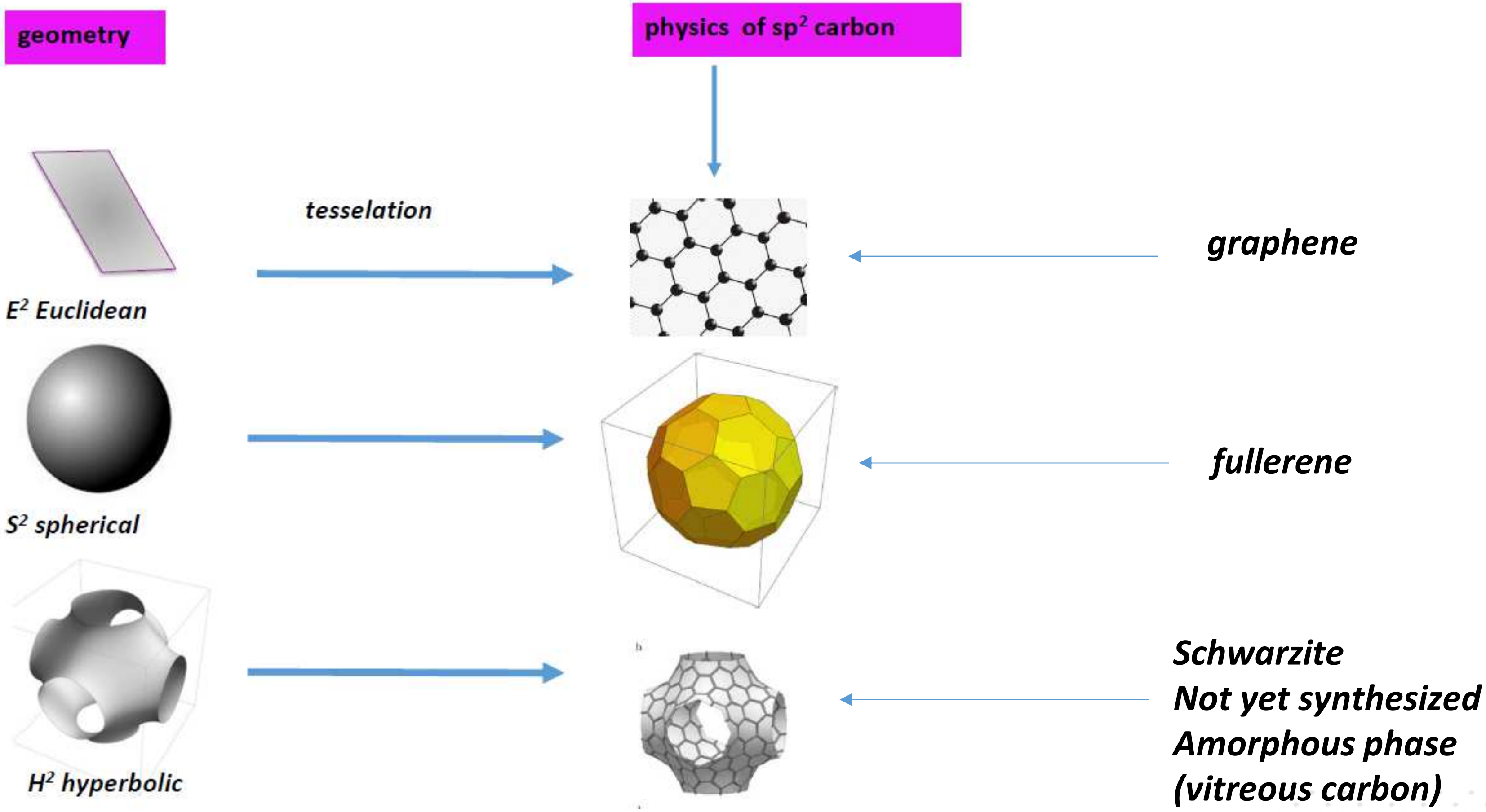
$$N_5 - N_7 - 2N_8 = 12(1 - g).$$

fullerene C_{60} g=0 N_7=N_8=0 then N_5=12

TPMS g≥3 the smaller one g=3 N_7=24

Extrinsic geometry (surface) Poincare uniformisation theorem

differential → *discrete*



Citation: Mélinon, P. Vitreous Carbon, Geometry and Topology: A Hollistic Approach. *Nanomaterials* **2021**, *11*, 1694. https://doi.org/10.3390/nano11071694

Figure 11. From continuous to discrete geometry in the three spaces: graphene (hexagon tiling), C_{60} (hexagon and pentagon tiling) and *TPMS* (hexagon and n-gon $n > 7$ tiling).

From differential to discrete geometry

topology: surface

In mathematics, a surface is a geometrical shape that resembles to a deformed plane.

topology describes the envelope

TESSELATION

topology= surface metric → *mathematical description polynomial form (continuous)* → *Grid (discrete)* → *Atomic coordinates: crystallography*

TOPOLOGY

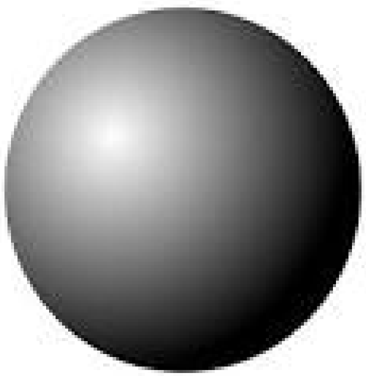
approximation

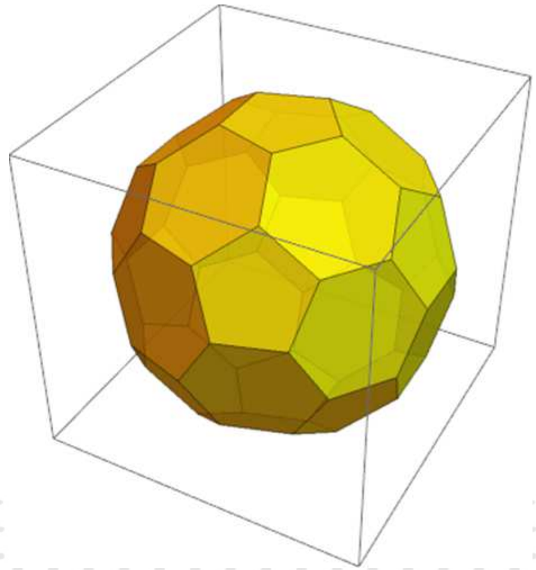
Weierstrass-Enneper Representation
Brakke's Surface Evolver

Hexagons
Pentagons
Heptagons…

Euler's rule

PHYSICS





pavement with a grid formed by hexagons/pentagons/ n-fold gons

Exemple: Schwarzites

Terrones, H.; Terrones, M. Curved nanostructured materials. *New J. Phys.* **2003**, *5*, 126.

Name	Space Group	d in Å	N	x	y	z
D688	$Pn\bar{3}m$ (224)	6.148	24	1:2	0.33342	0.66658
P688	$Im\bar{3}m$ (229)	7.828	48	0.31952	0.31952	0.09373
G688	$Ia\bar{3}d$ (230)	9.620	96	0.92205	0.12094	0.95502
gyroid	$Ia\bar{3}d$ (230)	18.599	384	0.18812	0.20968	0.77090
				0.07632	0.20151	0.84364
				0.02066	0.15594	0.87348

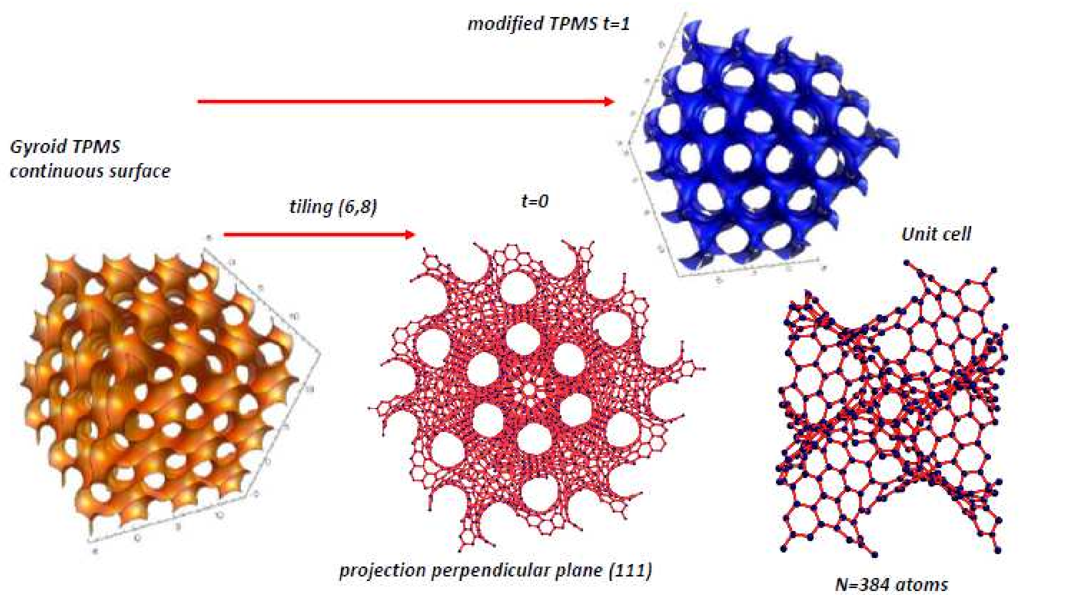


Figure 14. Gyroid *TPMS* with N = 384 atoms after tiling with hexagons and octagons (see Table 8, last line). The modified structure with $t = 1$ is discussed below.

(TPMS Triply Periodic Minimal surfaces)

H Mean curvature
K Gauss curvature (intrinsic)

H=0 K<0

genus 2≥3

hyperbolic geometry

A particular case: vitreous carbon : a piece of mystery

excellent biological compatibility with living tissues

high temperature resistance

hardness, low density, low electrical resistance

low friction

low thermal resistance

extreme resistance to chemical attack

impermeability to gases and liquids despite porosity !!!

and more…

A particular case: vitreous carbon : a piece of mystery

no consensus

but surface+holes

heptagons may be octogons and pentagons!

Thermodynamicaly Schwarzite synthesis is probably a dream

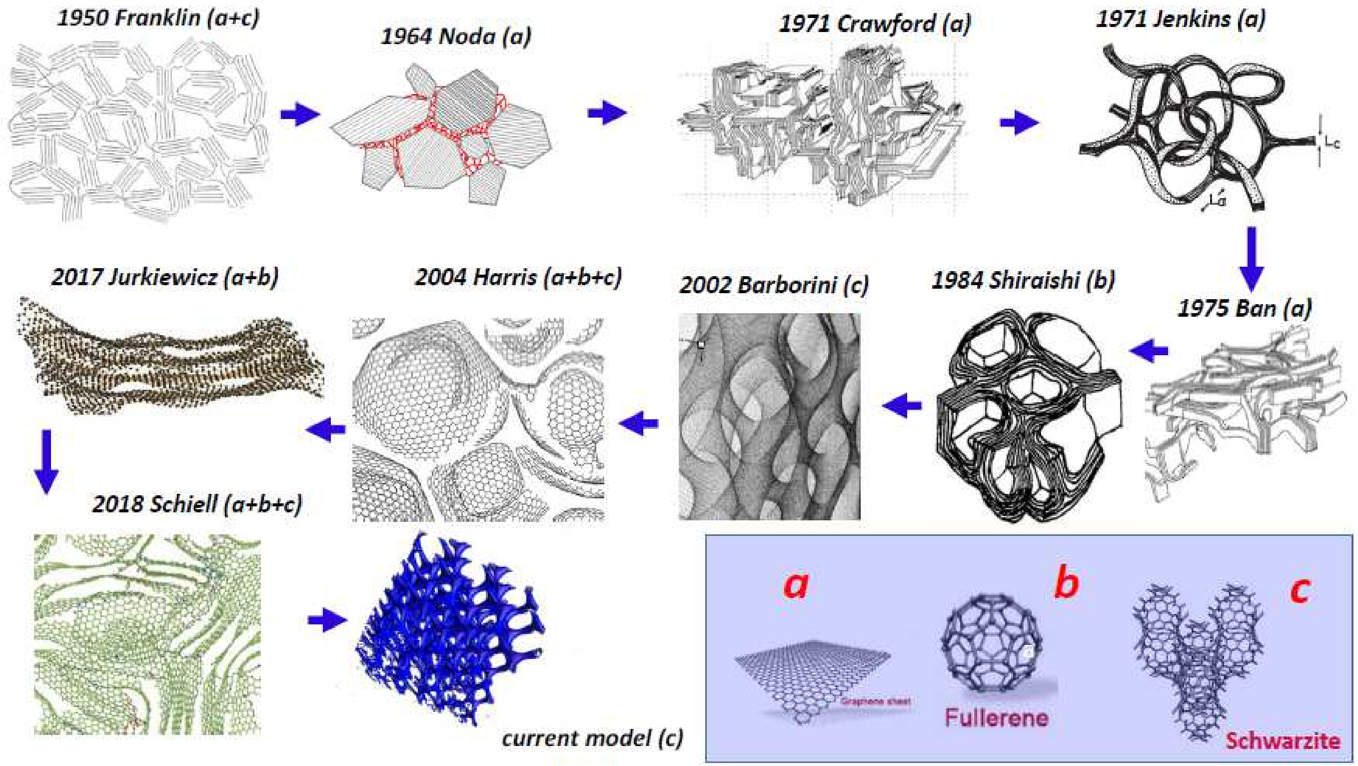


Figure 2. History and evolution of *GLC* throughout the ages, as presented by Franklin [7,8], Noda et al. [9], Crawford et al. [10], Jenkis et al. [12], Ban et al. [11], Shiraishi et al. [13], Barborini et al. [14], Harris [17], Jurkiewicz et al. [18] and Shiell et al. [20]. The insert (bottom right) shows the three elemental forms according to the curvature sign with labels a–c, respectively. The labels in the models correspond to the elemental bricks of the models. Figure 2 is adapted from [24]. Reproduced with permission from Shiell, Journal of Non-Crystalline Solids; copyright 2021, Elsevier.

vitreous carbon structure with holes

HRTEM (High Resolution Transmission Microscopy)
Vitreous carbon

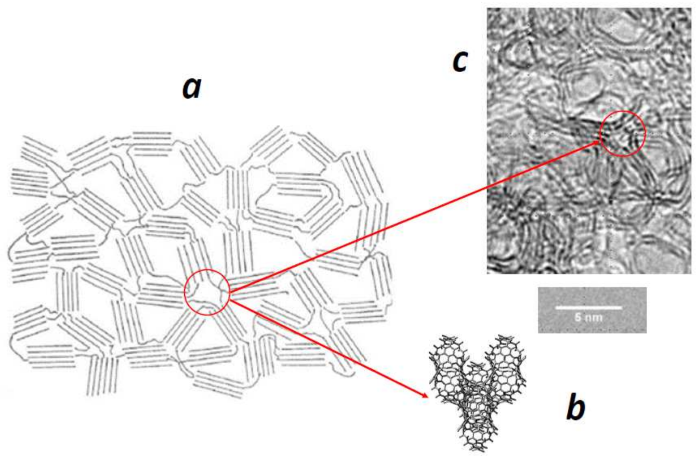


Figure 24. (**a**) Franklin's view of the *GLC*; (**b**) part of *HRTEM* pattern corresponding to the *GLC* produced by *PLD* and laser annealing (see Figure 5); and (**c**) an elemental cell of a Schwarzite *TPMS* structure [22].

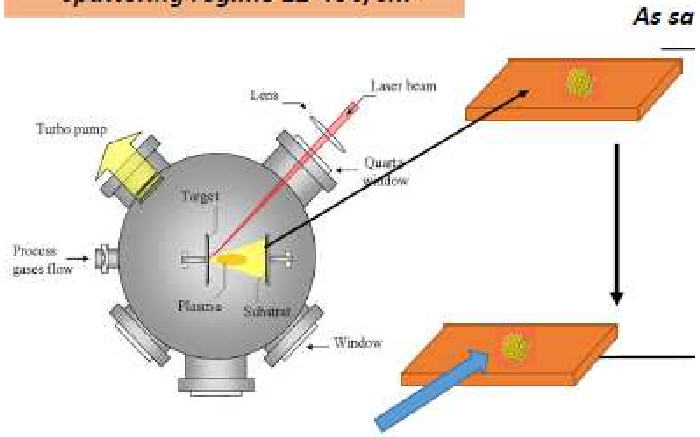
Schwarzites are the candidate

hyperbolic geometry opens the door

Physical route: laser ablation+ laser annealing

laser

λ = 248 nm, τ = 20 ns, f = 1-150 Hz
sputtering regime 12-40 J/cm^2



laser

λ = 248 nm, τ = 20 ns, f = 1-150 Hz
<< sputtering threshold : 0.15 J/cm^2

Chemical route: pyrolisis (T>2500K sugar…)

Stability in carbon structures

Graphene is the reference, stability is defined by the difference between the cohesive energy in the structure and the graphene (or diamond)

→ *Brut force + quantum chemistry calculation or DFT and beyond: exact but time (and money) consuming*

→ *POAV (Pi orbital Axis Vector)*

→ *Defect Formula: "Mathematical" Stability, orbifold (Thurston), Conway, Coxeter…*

→ *Willmore (differential geometry)*

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POAV geometrical model

« classical approach » chemistry

POAV: « π orbital axis vector » concept of rehybridization

$$\sin(\theta_{\pi\sigma} - \frac{\pi}{2}) = \frac{2\pi^{1/2}N^{-1/2}}{3^{3/4}},$$

the mean hybridisation n is written as

$$n = \frac{2}{1 - \frac{4\pi}{\sqrt{3}N}}$$

and the energy to graphene is given by a simple relationship

$$\Delta E(eV) = -3.1 \times 10^{-3}(\theta_{\pi\sigma} - \frac{\pi}{2})^2$$

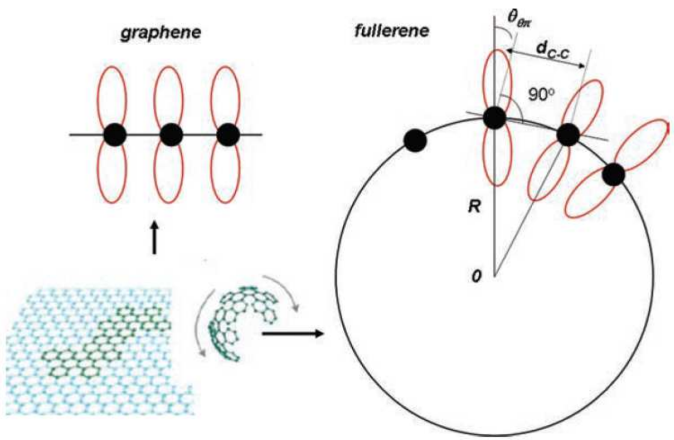


Figure 5.10. Misalignment of the π orbital when the graphene plane is curved.

Defect formula

Orbifold (Conway, Thurston) symmetry groups in two-dimensional spaces of constant curvature

The orbifold of such a group is "the surface divided by the group"

The local Gauss–Bonnet theorem relates the curvature integrated over the surface area within a surface patch P bounded by a p-sided polygon with geodesic edges

Gauss Bonnet (discrete)

$$\chi_{loc} = (2-p)\pi + \sum_{i=1}^{p} v_i$$

internal vertex angles v_i

p-sided polygon

Hyde et al Acta Crystallogr. Sect. A Found. Adv. 2014, 70, 319–337

Table 4. Isometry (symmetry operator), orbifold symbol and associated Euler characteristic χ^i_{loc}. All orbifolds contain a foundation sphere [70].

Isometry	Orbifold Symbol	χ^i_{loc}
(sphere)	1	2
pair of translations	o	-2
rotation centre	A	(1-A)/A
reflection line	*	-1
rotoreflection	(*) i	(1-i)/2i
glide line	x	-1

structure (graphene, fullerene…)
List of isometries

$$\chi_0 = 2 - \sum_{orbifold\, i} \chi^i_{loc}$$

stability needs minimization of χ_0

defect formula

Table 5. Isometries of $\mathbb{E}^2$ limited to the Coxeter class (for the definition, see [74]). χ_o is the fractional Euler characteristic (see Section 5.7.2) [70]. (finite Euclidean reflection groups)

Isometry	Orbifold Symbol	Group Number	χ_o
*632	p6m	17	0
*333	p3m1	14	0
*442	p4m	11	0
*2222	pmm	6	0

graphene

Table 6. Isometries of $\mathbb{S}^2$ limited to the Coxeter class. χ_o is the fractional Euler characteristic (see Section 5.7.2) [70].

Isometry	Orbifold Symbol	Group Number	χ_o
*235	-	-	1/60
*234	m3m	221–230	1/24
*233	$\bar{4}$3m	215–220	1/12
*22k	-	-	1/2k
*226	6/mmm	191–194	1/12
*224	4/mmm	123–142	1/8
*223	$\bar{6}$2m	189	1/6
*222	mmm	47–74	1/4
*kk	-	-	1/k
*66	6mm	183	1/6
*44	4mm	99–110	1/4
*33	3m	156–161	1/3
*22	mm2	25–46	1/2
*	m	6–9	1

fullerene

Table 7. Isometries of $\mathbb{H}^2$ limited to the Coxeter class and $\chi_o > -1/12$. χ_o is the fractional Euler characteristic (see Section 5.7.2). Negative characteristics correspond to groups acting in the hyperbolic plane [70].

Orbifold Symbol	χ_o
*237	−1/84
*238	−1/48
*245	−1/40
*239	−1/36
*23 (10)	−1/30
*23 (11)	−5/132
*23 (12), *246, *334	−1/24

TPMS

stability $E_{graphene} > E_{fullerene} > E_{TPMS}$

Benedek et al The Topological Background of Schwarzite Physics

Table 12.1 Cohesive energy per atom (E_{coh}), density, bulk modulus (**B**), bond strength (**b**) and conductive property for the smallest D-type schwarzites with tetrahedral symmetry, as compared to fullerite and diamond (Gaito et al. 2001; Benedek et al. 1997, 2001)

D-type schwarzite	E_{coh} (eV/atom)	Density (g/cm^3)	B (Mbar)	b (Mbar Å^3)	
fcc-$(C_{28})_2$	−7.66	1.33	1.58	16.12	Metal
fcc-$(C_{36})_2$	−7.71	1.05	1.26	16.20	Insulator
fcc-$(C_{40})_2$	−7.92	1.60	1.92	16.25	Metal
fullerite	−7.99	1.71	0.14	–	Insulator
diamond	−8.36	3.52	4.42	16.71	Insulator
graphite	-8.37				

defect formula in agreement with full calculations

Institut Lumière Matière

summary: carbon molecules in terms of « orbifolds »

Huson, D. Two-Dimensional Symmetry Mutation 1991.

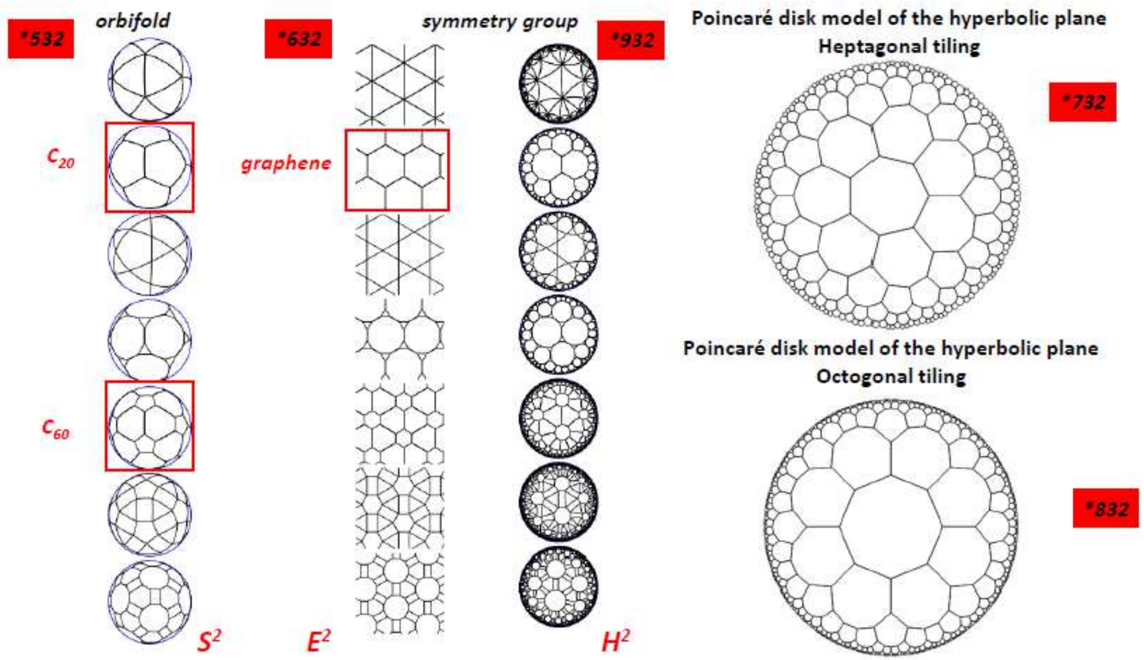


Figure 12. (**left**) Different orbifold (symmetry group, 532*, 632* and 932*) corresponding to $\mathbb{E}^2$, $\mathbb{S}^2$ and $\mathbb{H}^2$, respectively. The two fullerenes C_{20} (I_h) and C_{60} (I_h) belong to the 532* symmetry group. Graphene belongs to the 632* symmetry group [76]. (**right**) Poincaré disk model of the hyperbolic plane showing the tiling with heptagons or octagons (Platonic tessellation). The case of octagon tiling corresponds to the double torus in Figure 9.

Willmore

compact oriented surface S embedded in $\mathbb{R}^3$,

a and b are related to the flexural bending rigidity and bending stiffness

$$H(S) = a\int_S H^2 dA + b\int_S K dA$$

$\nu = 1 + \frac{a}{b}$ ***Poisson ratio***

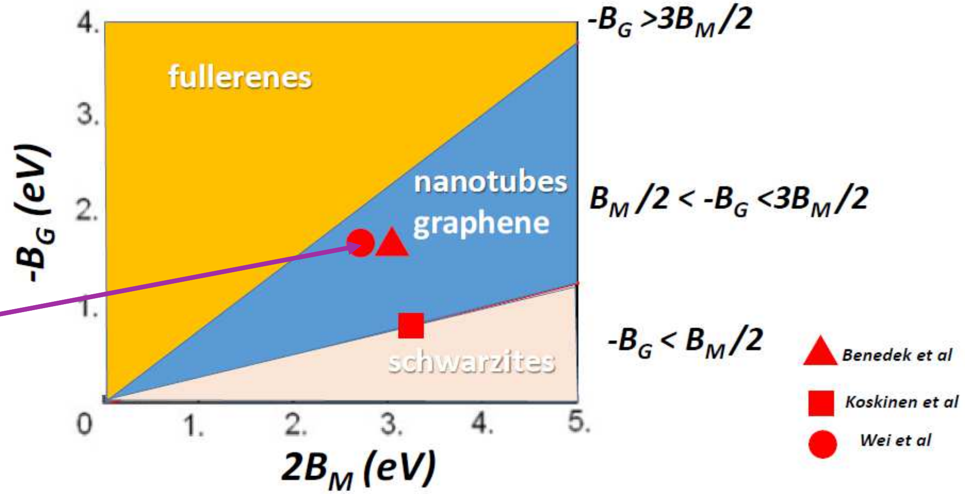
$a = -b$ ***Willmore***

$$H(S) = \int_S (2B_M H^2 + B_G K) dA$$

B_M and B_G are the bending rigidity and the Gaussian bending

$$B_M = 1.44\,\text{eV and } B_G = -1.52\,\text{eV}$$

(DFT calculations)



other data are available! no consensus for B_M and B_G

Benedek, G.; Bernasconi, M.; Cinquanta, E.; D'Alessio, L.; De Corato, M. The topological background of schwarzite physics. InThe Mathematics and Topology of Fullerenes; Springer: Berlin/Heidelberg, Germany, 2011; pp. 217–247.

Summary: cohesive energy fullerenes to graphene

Fullerenes

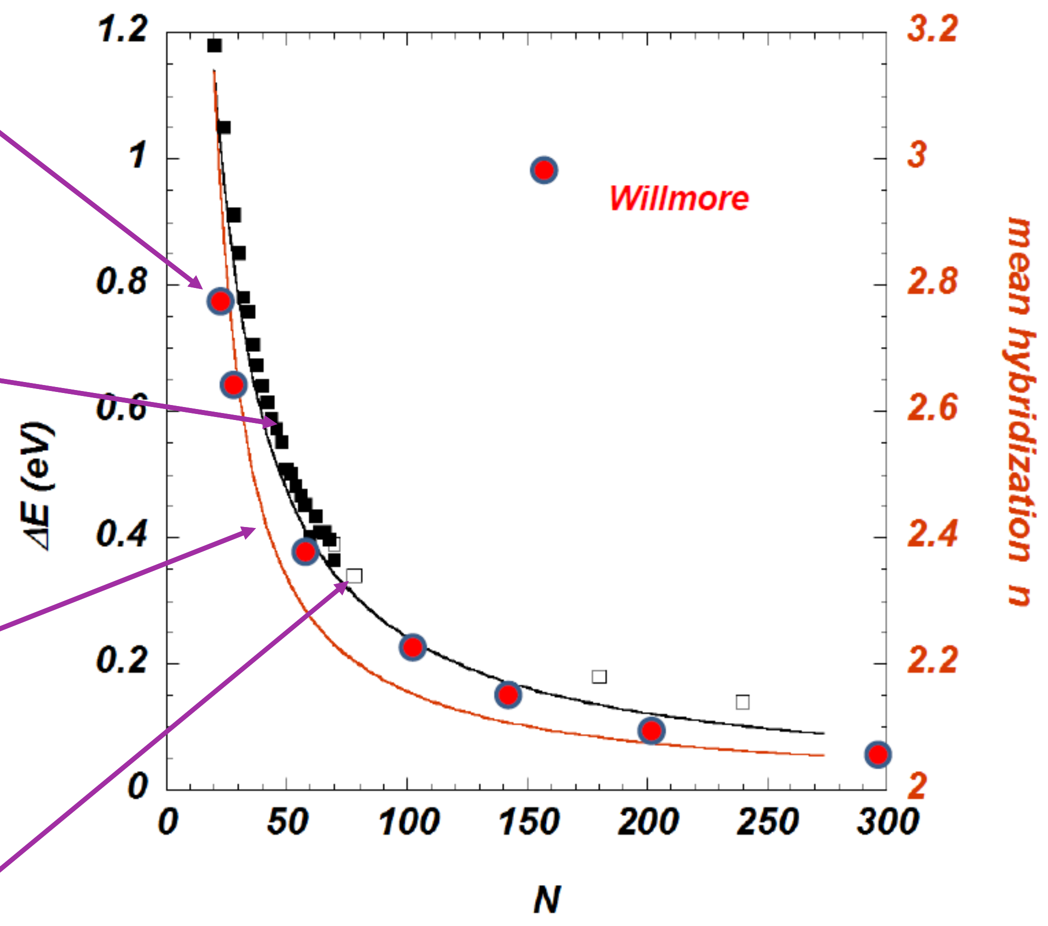
S^2 spherical

Willmore

Ab Initio DFT

POAV

Semi Ab Initio DFT+ tight binding



Conclusion and open issues

topology

Work is in progress

- *understand some amazing properties (graphene, topological insulators…)* « Monitoring » the periodicity
- *toolbox for kinetics (topological invariants are preserved)*
- *Fermion (electron) base space+ fiber (bundle) space (trivial versus non trivial), boson (phonon) torus anyway*

open

- *non orientable structures (real projective surfaces…)* $\mathbb{R}^3 \longrightarrow \mathbb{R}^4$
- *topology applied to physical problems (impurities in periodic cells versus impurities in torus)*

geometry

Work is in progress

- *stability of carbon structures*

Hyperbolic geometry

open

- *Fractal structures (example Hadamar walk in Sierpinsky carpet)*
- *Chaotic motion « fuite de Poincaré «*
- *Mechanical properties (macroscopic to microscopic) differential to discrete geometries*

An example where topology improves results: Madelung constant

Clifford boundary conditions: a simple direct-sum evaluation of Madelung constants

Nicolas Tavernier,[1] Gian Luigi Bendazzoli,[2] Véronique Brumas,[1] Stefano Evangelisti,[1,*] and J. A. Berger[1,3,†]
[1] *Laboratoire de Chimie et Physique Quantiques, IRSAMC, CNRS, Université de Toulouse, UPS, France*
[2] *Università di Bologna, Bologna, Italy*
[3] *European Theoretical Spectroscopy Facility (ETSF)*
(Dated: July 23, 2020)

We propose a simple direct-sum method for the efficient evaluation of lattice sums in periodic solids. It consists of two main principles: i) the creation of a supercell that has the topology of a Clifford torus, which is a flat, finite and border-less manifold; ii) the renormalization of the distance between two points on the Clifford torus by defining it as the Euclidean distance in the embedding space of the Clifford torus. Our approach does not require any integral transformations nor any renormalization of the charges. We illustrate our approach by applying it to the calculation of the Madelung constants of ionic crystals. We show that the convergence towards the system of infinite size is monotonic, which allows for a straightforward extrapolation of the Madelung constant. We are able to recover the Madelung constants with a remarkable accuracy, and at an almost negligible computational cost, i.e., a few seconds on a laptop computer.

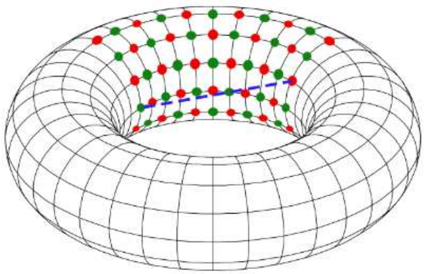


FIG. 1. An illustration of a Clifford supercell for a 2-dimensional NaCl structure; red dots represent Na^+ and green dots represent Cl^-. The dashed blue line indicates the renormalized distance between two ions in the Coulomb potential. It is the shortest distance in the embedding space of the torus. We note that a true Clifford torus has a flat surface which is impossible to represent graphically.

ESC direct: cube replica
Ejven renormalization with different fractional fictive charges

CSC Clifford

TABLE II. The Madelung constant of Cs^+ in CsCl for various values of K, the number of unit cells per side. The extrapolated $K \to \infty$ value has been obtained through a linear fit in K^{-2} according to Eq. (14) using the CSC results that correspond to the two largest K values.

K	ESC	Evjen	CSC
40	-165.1951301706	-3.1228159774	-1.7613129129
41	-172.8428945898	-0.4025235314	-1.7613786888
42	-173.4399599212	-3.1228353436	-1.7614398086
43	-181.0877243486	-0.4025055166	-1.7614967019
60	-247.6434281092	-3.1229317065	-1.7620703281
80	-330.0917264008	-3.1229722138	-1.7623349348
100	-412.5400247666	-3.1229909632	-1.7624573245
120	-494.9883231553	-3.1230011482	-1.7625237851
∞			-1.7626748322

Reference value: [21] -1.7626747731

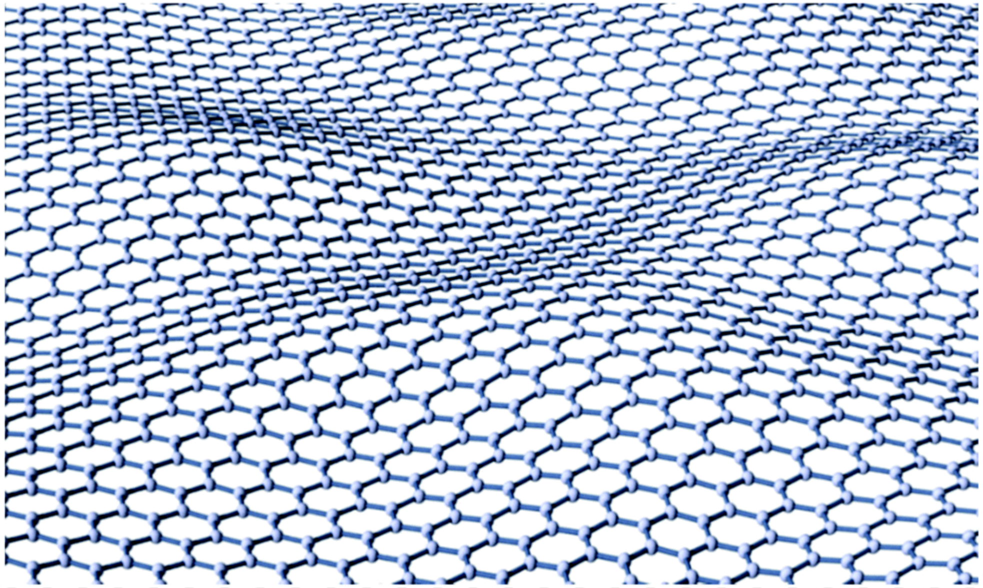
When mathematics confronted with the reality

Mermin-Wagner theorem (short range order)

but

2D infinite sheets are no stable at T≠ 0 k

ripples are observed in graphene at long range order

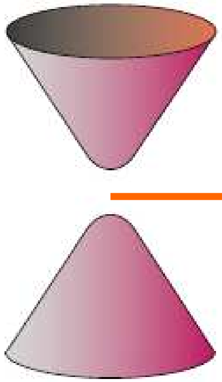


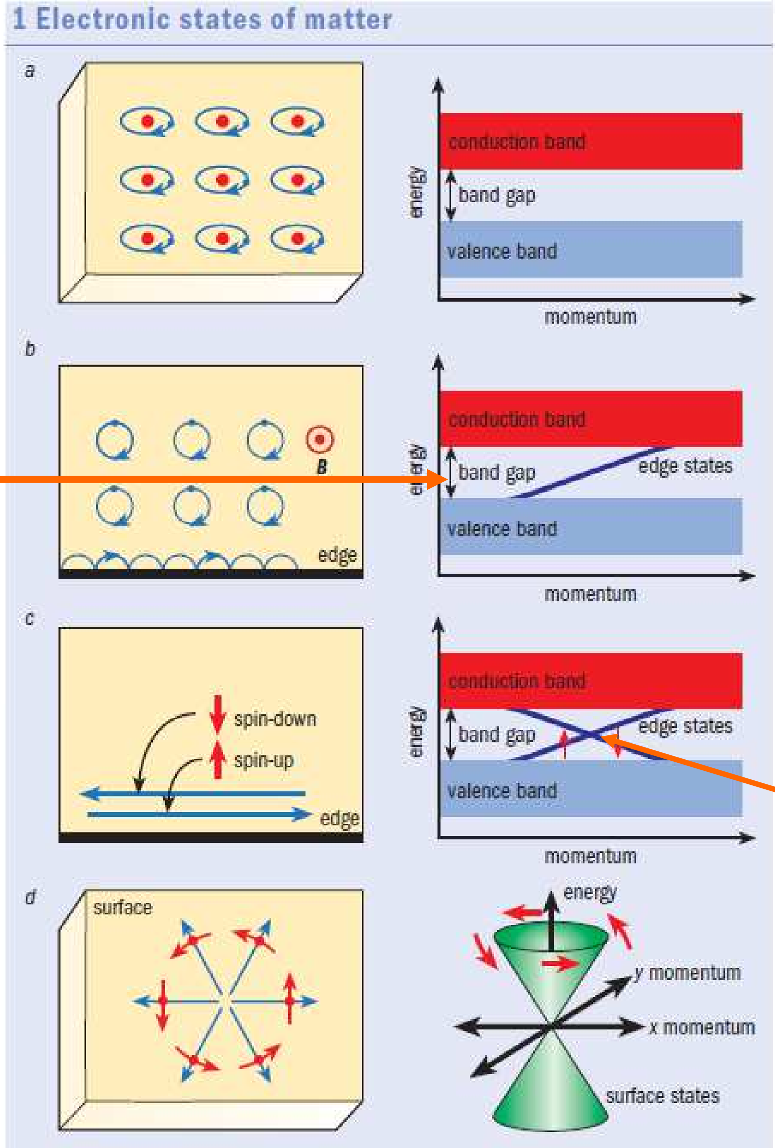
Jahn Teller theorem

"any molecule or complex ion in an electronically degenerate state (excepted spin) will be unstable relative to a configuration of lower symmetry in which the degeneracy is absent".

↓

spontaneous symmetry breakdown





An interface between different topological states has topologically protected midgap states

insulator

Topological gapped phases

Magnetic field (current)

graphene

With spin orbit (no net current) graphene with spin orbit

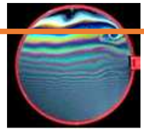
gapless

3D Nielsen-Ninomiya theorem, aka fermion-doubling theorem:

Hasan, M. Z., & Kane, C. L. (2010). Colloquium: topological insulators. *Reviews of modern physics*, *82*(4), 3045.

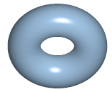
Modèle structural du carbone vitreux

Aspect topologique:



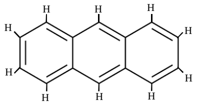
$g = 0$

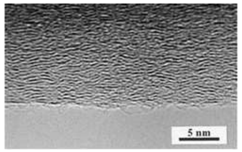
$g = 1$



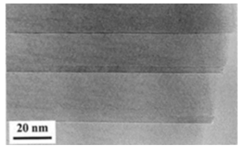
Composé organique $\xrightarrow{\text{pyrolyse}}$ Carbone graphitisable ou non graphitisable

Anthracène $C_{14}H_{10}$



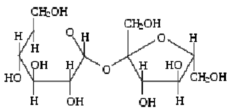


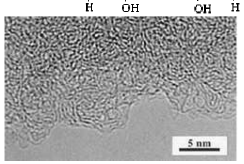
graphite



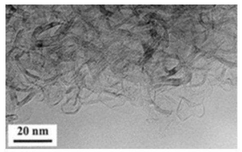
$g = 0$

Sucrose $C_{12}H_{22}O_{11}$





carbone vitreux

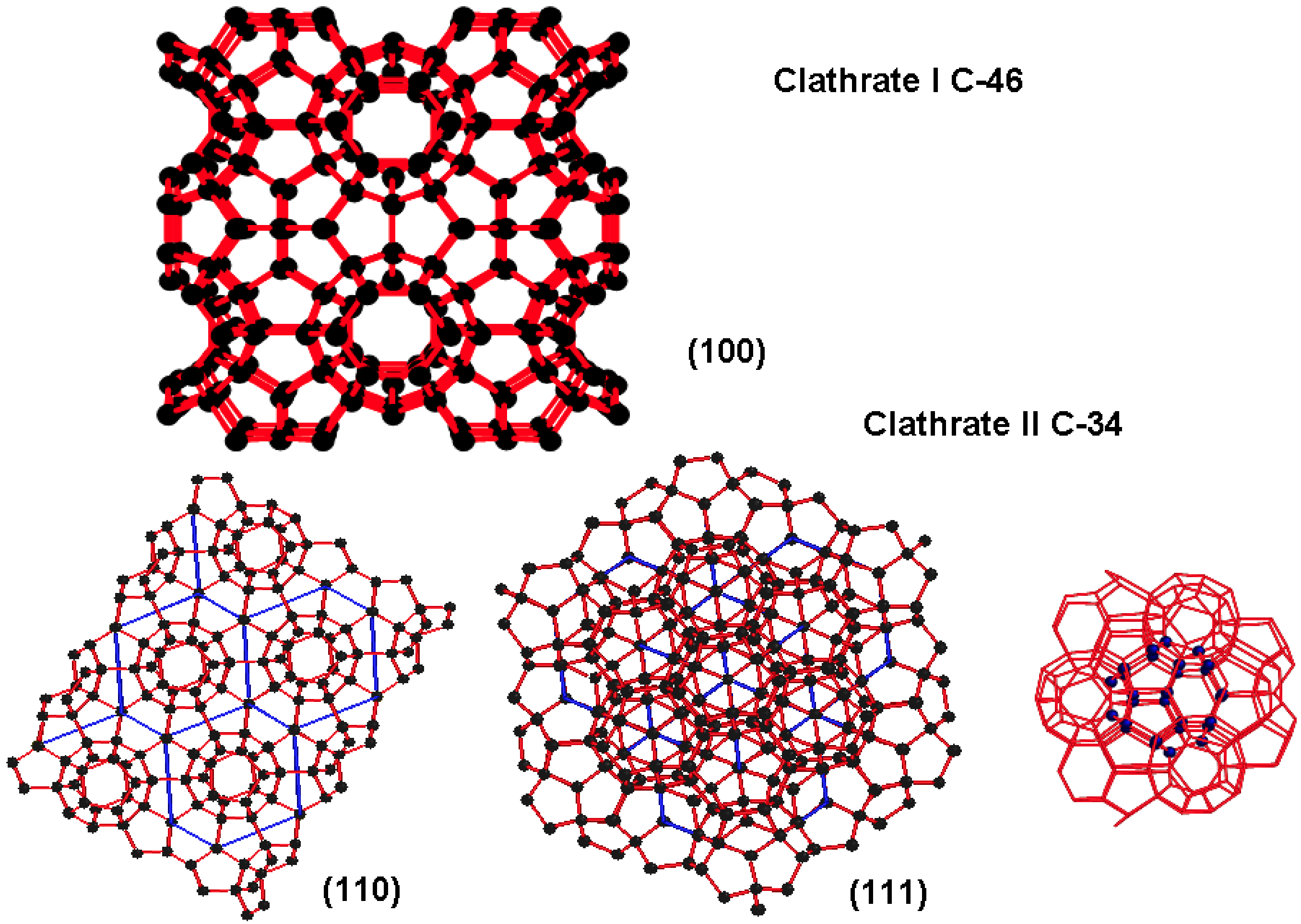


$g \geq 3$

Autre Composés non graphitisables: chlorure de polyvinylidène $C_2H_2Cl_2$
Autre Composé graphitisable: chlorure de polyvinyle C_2H_2Cl

Même éléments chimiques
mais
d'invariant topologique ≠

Invariant topologique ≥ 3 = clef de la synthèse du carbone vitreux!


Clathrate I C-46
(100)
Clathrate II C-34
(110)
(111)

any stress tensor can be decomposed into the sum of hydrostatic and deviatoric stresses as follows

$$\sigma_{ij} = \frac{1}{3}\delta_{ij}\sigma_{kk} + \sigma'_{ij}$$

Von Mises

$$\sigma_{\mathrm{VM}} = \sqrt{\frac{3}{2}\sigma_{ij}\sigma_{ij} - \frac{1}{2}(\sigma_{kk})^2}$$

shape

an **isotropic** and **ductile** metal will yield when subjected to a complex loading condition.

The same is true for strain.

$$\epsilon_{ij} = \frac{1}{3}\delta_{ij}\epsilon_{kk} + \epsilon'_{ij}$$

where $\frac{1}{3}\delta_{ij}\epsilon_{kk}$ is the hydrostatic term and ϵ' is the deviatoric strain.

, **Poisson's ratio** ν (nu) is a measure of the **Poisson effect**, the deformation (expansion or contraction) of a material in directions perpendicular to the specific direction of loading.

For open-cell polymer foams, Poisson's ratio is near zero, since the cells tend to collapse in compression.

The symmetry operators in graphene are, respectively, a reflection line (orbifold symbol *, $\chi^i_{loc} = 1$) and three rotation centres with angles $\pi/6$ ($\chi^i_{loc} = 5/12$), $\pi/3$ ($\chi^i_{loc} = 2/6$) and $\pi/2$ ($\chi^i_{loc} = 1/4$) (orbifold symbols 6, 3 and 2, respectively). Using Table 4, Equation (29) gives (see Table 7)

$$\chi_o(graphene) = 2 + (-1 - 5/12 - 2/6 - 1/4) = 0 \tag{30}$$

$\mathbb{S}^2$, giving a symmetric pattern with identical vertices defined by a spherical triangular asymmetric domain, with 2, 3 and 5 mirror lines meeting at each vertex. The Coxeter orbifold is *235 or equivalently, the I_h point group in classical crystallography in $\mathbb{E}^3$. Then

$$\chi_0(C_{60}) = 2 + (-1 - 1/4 - 1/3 - 2/5) = +1/60 \tag{31}$$

Table 4. Isometry (symmetry operator), orbifold symbol and associated Euler characteristic χ^i_{loc}. All orbifolds contain a foundation sphere [70].

Isometry	Orbifold Symbol	χ^i_{loc}
(sphere)	1	2
pair of translations	o	-2
rotation centre	A	(1-A)/A
reflection line	*	-1
rotoreflection	(*) i	(1-i)/2i
glide line	x	-1