CHEMICAL GRAPH THEORY

- Pictorial Introduction

Part 4

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When $d=3$ and $k=7/3$ the polynomial-like Wiener index assumes the form:

$$W(N) = a_7N^{7/3} + a_6N^{6/3} + a_5N^{5/3} + \ldots + a_1N^{1/3} + a_0$$

By posing $Y = N^{1/3}$

$$W(N) = a_7Y^7 + a_6Y^6 + a_5Y^5 + \ldots + a_1Y + a_0$$

we have a truly polynomial Wiener index growing term ruled in the limit $N \to \infty$ by $W(N) \approx a_7Y^7$
DISTANCE BASED GRAPH INVARIANTS IN INFINITE 3D-SYSTEMS

Does $Y=N^{1/3}$ possess any structural meaning?

If we have a $L \times L \times L$ simply cubic lattice $N = L^3$.
$L=3$ in this case $N=27$.

NOTE Each cubic cell has 1 atom.

Then as $L$, $Y$ gives the number of cell along each axis of the structure.

Exercise: write the relations $N$ and $L^3$ and $Y$ and $N$ when the unit cell has $n_0$ atoms.
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- An important research topic at our LAB

CARBON BASED BULK 3D SYSTEM

SCHWARZITZES
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- **SCHWARZITITES** have bulk structure, not flat like in PAH, graphene, nanotubes, nor hollow like in and fullerenes nanocone.

- How this is possible with sp²-carbon atoms?
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- **SCHWARZITES HAVE BULK STRUCTURE**

- How this is possible with sp²-carbon atoms?

- Remember we induce a positive curvature in the plane by adding 1 pentagon:

- Producing a nano...? And then a fu....?

- ANY IDEA TO INDUCE NEGATIVE CURVATURE?
SCHWARZITES HAVE BULK STRUCTURE

How this is possible with \( sp^2 \)-carbon atoms?

We induce a NEGATIVE curvature in the plane by adding 1 HEPTAGON
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- SCHWARZITES HAVE BULK STRUCTURE
- How this is possible with sp² -carbon atoms?
- MATH and Nature both love NEGATIVE curvature
TOPOLOGICAL INDICES WORK also for CARBON BASED BULK 3D SYSTEM

Example:
Stability of single atoms in SCHWARZITIC INFINITE LATTICES

<table>
<thead>
<tr>
<th>W</th>
<th>Average d (Å)</th>
</tr>
</thead>
<tbody>
<tr>
<td>172.5</td>
<td>1,408</td>
</tr>
<tr>
<td>173</td>
<td>1,415</td>
</tr>
<tr>
<td>174</td>
<td>1,494</td>
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<tr>
<td>174.5</td>
<td>1,455</td>
</tr>
<tr>
<td>176</td>
<td>1,522</td>
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</tbody>
</table>
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see:
Electronic properties of curved graphene sheets
Alberto Cortijo, María A. H. Vozmediano
Universidad Carlos III de Madrid-ICMMeoqusy


And web pages
http://hyperbolic-crochet.blogspot.ro/2012_07_01_archive.html

http://westy31.home.xs4all.nl/Geometry/Geometry.html
DISTANCE BASED GRAPH INVARIANTS IN INFINITE DEFECTIVE SYSTEMS

- THIS IS ANOTHER IMPORTANT SECTOR FOR OUR LAB RESEARCHES - WE INTRODUCE TOPOLOGICAL DEFECTS BY ROTATING ONE BOND

- DID YOU THINK PERHAPS TO CURVATURE?
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- THIS BOND ROTATION IS CALLED STONE-WALES ROTATION OR REARRANGEMENT OR FLIP OR TRANSFORMATION

Exercise: compute Distance Matrix and $W(N)$ for the 2 molecules
IN OUR LAB WE STUDY THE EFFECT OF THE DEFECTS ON LATTICE STABILITY SEARCHING FOR THE SIZE OF THE NANOSTRUCTURE FOR WHICH THESE DEFECTS ARE STABLE. OUR RESULT 15-30 Å IS IN AGREEMENT WITH AB-INITIO SIMULATION
Topological potentials are capable to simulate effectively long-range mechanism responsible for phase transitions in 1D systems.

Long-range information stored in the topological structure or invariants of (large) systems greatly dominate their properties.

In particular, delocalized behaviors of the topological picture “naturally” fit in the picture of the BONDON, the bosonic new particle - Prof. PUTZ’s original idea - corresponding to the chemical bond field.

Future work is planned to assessing an experimental signature to this boson.
Topological potentials represent from one side a very strong approximation of reality BUT they have a good capacity to simulate reality. How we may improve them?

OUR STRATEGY I TO COLOR THE GRAPH WITH NUMBERS COMING FROM AB-INITIO ELECTRONIC INFORMATION

The so-called TIMISOARA-PARMA rule
The so-called TIMISOARA-PARMA rule assigns the axial distribution of electronegativity and chemical hardness to a given molecular structure based on the (CFD) hierarchy.

In this way for example the pentacene graph gets full of color expressing the role each group of atoms has in determine properties like molecular reactivity, toxicity etc.
The indices like $W(N)$ became a bit more complex in the colored versions but retain their matrix form then they remain easy to manage.

$$W(\chi) = \det^{1/N_\pi} \left| \hat{W}_\chi \right|$$

$$w(\chi)_{ij} = \left[ \hat{W}_\chi \right]_{ij} = \left( \prod_{\alpha} \chi_\alpha \right)^{1/(1+d_{ij})}$$

$$W(\eta) = \det^{1/N_\pi} \left| \hat{W}_\eta \right|$$

$$w(\eta)_{ij} = \left[ \hat{W}_\eta \right]_{ij} = \left( \prod_{\alpha} \eta_\alpha \right)^{1/(1+d_{ij})}$$
The new colored indices carry the reactivity information in a very efficient way and they are called for that TOPO-REACTIVITY INDICES.

For a large set of PAH’s their behavior has been proofed to be the correct one.
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see:


Parabolic Reactivity “Coloring” Molecular Topology: Application to Carcinogenic PAHs Mihai V. Putz, Ottorino Ori, Franco Cataldo, Ana-Maria Putz Current Organic Chemistry, 2013, 17, 2816-2830

AND RELATED REFERENCES
MANY THANKS
FOR YOUR
ATTENTION

Questions ?

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