Forging graphene pseudospheres to mimic curved space–times

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Trento, 25/07/2019

Outline

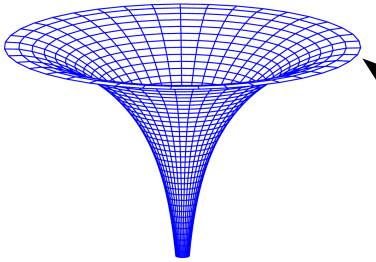
I. Introduction to the theoretical model – aim of the work;

II. Methods, Computational details & Results of the modeled carbon structures;

III. Methods, Computational details & Results of the electronic properties of such structures;

IV. Conclusions and discussions.

I. Theoretical framework



Hilbert Horizon ≈ Rindler horizon

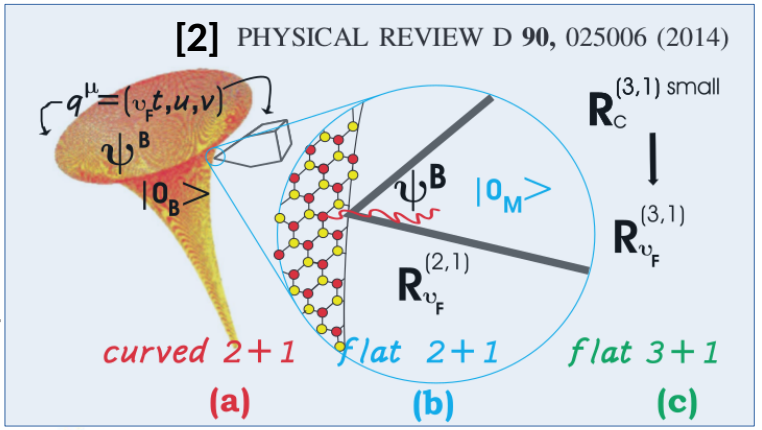
This work stems from the idea that a graphene monolayer arranged in a Beltrami pseudosphere shape can be used to realize a realistic analogue of a quantum field in a curved spacetime [1,2,3].

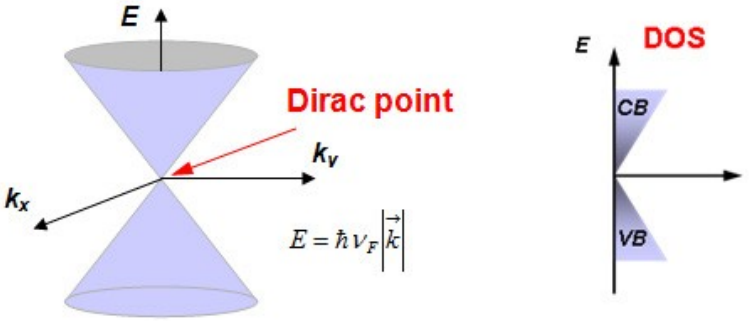
In particular it is shown [1,2] that curved graphene can be used to test the physics of the *Hawking-Unruh effect*.

↓

Analytical results [1,2] predict a thermal spectrum revealed through a characteristic electronic local density of states (LDOS)

This property derives from the unique electronic properties of graphene at the BZ Dirac points.





[1] A. Iorio, G. Lambiase, *The Hawking-Unruh phenomenon on graphene*, Phys. Let. B 716 (2), September 2012

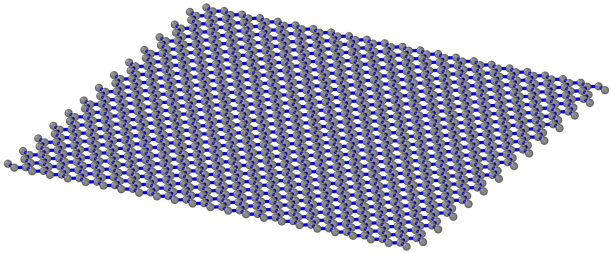
[2] A. Iorio, G. Lambiase, *Quantum field theory in curved graphene spacetimes, Lobachevsky geometry, Weyl symmetry, Hawking effect, and all that*, Phys. Rev. D 90, 025006, July 2014

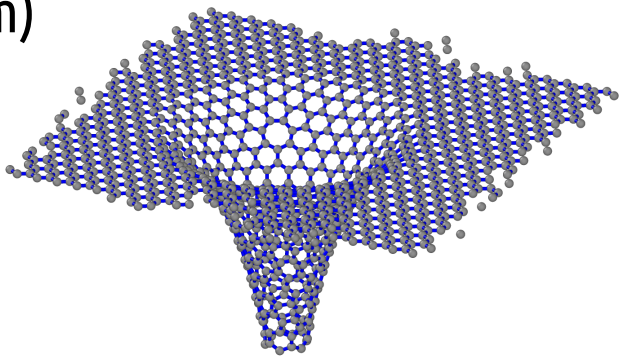
[3] S. Taioli et al., *Lobachevsky crystallography made real through carbon pseudospheres*, J. Phys.: Condens. Matter 28, 2016

I. Aim of the work

The goal of this study is to perform a computational "experiment" to reproduce in a discretized space the analytical results obtained in a continuum manifold [1,2].
This is achieved in two steps:

i) **By building a geometrical model of sp^2 carbon atoms arranged as in graphene placed on a Beltrami pseudosphere of radius $R \geq 10^2$ nm - accomplished** (within the approximations done in [1,2], we need to reach a ratio $R/l >> 1$ where $l=0.142$ nm)





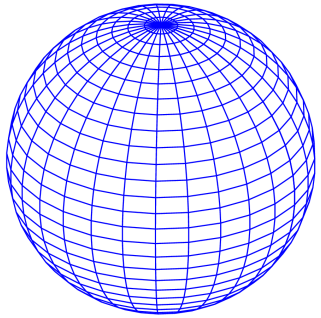
ii) **By computing the LDOS of this structure to study how the intrinsic curvature modifies the electronic behaviour of graphene – accomplished (but still difficulties in the interpretation of results)**

[1] A. Iorio, G. Lambiase, *The Hawking-Unruh phenomenon on graphene*, Phys. Let. B 716 (2), September 2012

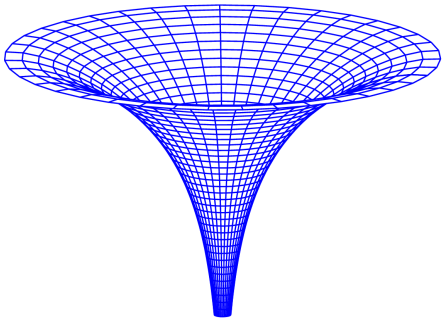
[2] A. Iorio, G. Lambiase, *Quantum field theory in curved graphene spacetimes, Lobachevsky geometry, Weyl symmetry, Hawking effect, and all that*, Phys. Rev. D 90, 025006, July 2014

II. Building carbon pseudospheres

$K = 1/R^2$	$K = -1/R^2$
$u \in [-\pi/2,\pi/2]$; $v \in [0,2\pi]$	$u \in [-\infty,0]$; $v \in [0,2\pi]$
$x(u,v)=R*\sin(u)*\cos(v)$	$x(u,v)=c*e^{u/R}*\cos(v)$
$x(u,v)=R*\sin(u)*\sin(v)$	$y(u,v)=c*e^{u/R}*\sin(v)$
$z(u)=R*\cos(u)$	$z(u)=R*(1-c*e^{2u/R}/R^2)^{1/2}$ $-\text{atanh}(1-c*e^{2u/R}/R^2)^{1/2}$



Carbon atoms on a sphere: ***fullerene***



Carbon atoms on a pseudosphere: ***???***

Gauss-Bonnet theorem: $2\pi\chi = K_{tot} + \int_{\partial\Sigma} K_g\, dl$

χ : *Euler characteristic*

K_{tot}: *total Gaussian curvature of the* Σ *surface*

To model the structure we build a 3-connected ***graph*** (N,L,F) of N vertices, L edges and F faces.

We store all the information on bonds and faces of the graph.

Best energy configuration of vertices, interacting through a Keating potential: Wooten, Winer, Weaire (WWW) method [4].

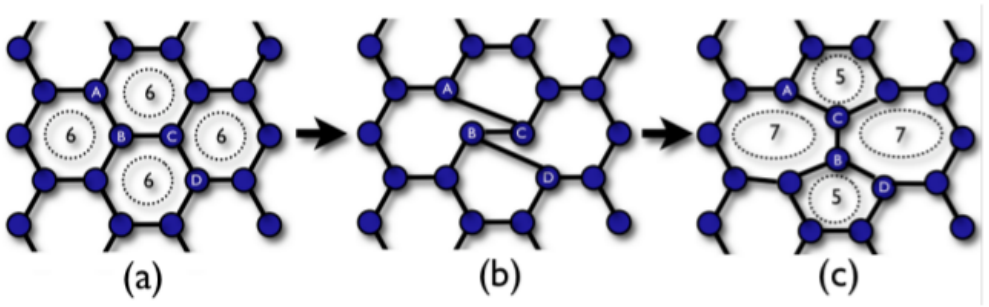
$$E = \frac{3}{16}\frac{\alpha}{l^2}\sum_{i,j}\left(r_{ij}^2 - l^2\right)^2 + \frac{3}{8}\frac{\beta}{l^2}\sum_{i,j,k}\left(\vec{r}_{ij}\cdot\vec{r}_{ik} - l^2/2\right)^2$$

2-body part **3-body part**

[4] F. Wooten, K. Winer, and D. Weaire, *Computer Generation of Structural Models of Amorphous Si and Ge*, Phys. Rev. Lett. 54 (1392), April 1985

II. Building carbon pseudospheres

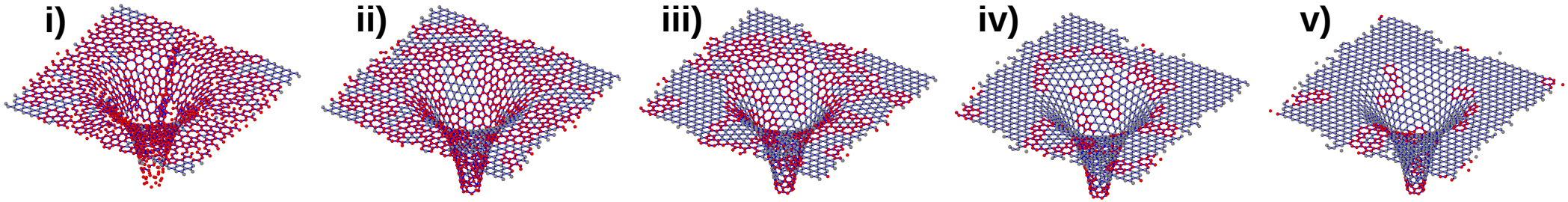
The minimum is found by switching bonds between atoms with a Monte Carlo algorithm, accepting the trial switches with a Metropolis probability, and iterating until the total energy does not decrease any more.



[5]

At every step, *minimizations* - and *structural relaxations* - were carried out using FIRE (Fast Inertial Relaxation Engine for optimization on all scales) [6] algorithm.

An example of how our method works



Snapshots taken during the optimization procedure (every ~ 2000 trial switches)

Atoms not belonging to hexagonal faces only are highlighted in red

[5] S. V. Alfthan, *Computational studies of silicon interfaces and amorphous silica*, PhD Thesis, Helsinki University of Technology

[6] E. Bitzek et al., *Structural relaxation made simple*, Phys. Rev. Lett. 97 (170201), October 2006

II. Building carbon pseudospheres

We perform several simulations starting from different initial number of atoms (vertices).

Problem: the method works well (reasonable time) for systems with number of atoms ≤ 3000 (R of the order of 3 nm). How to increase dimensions?

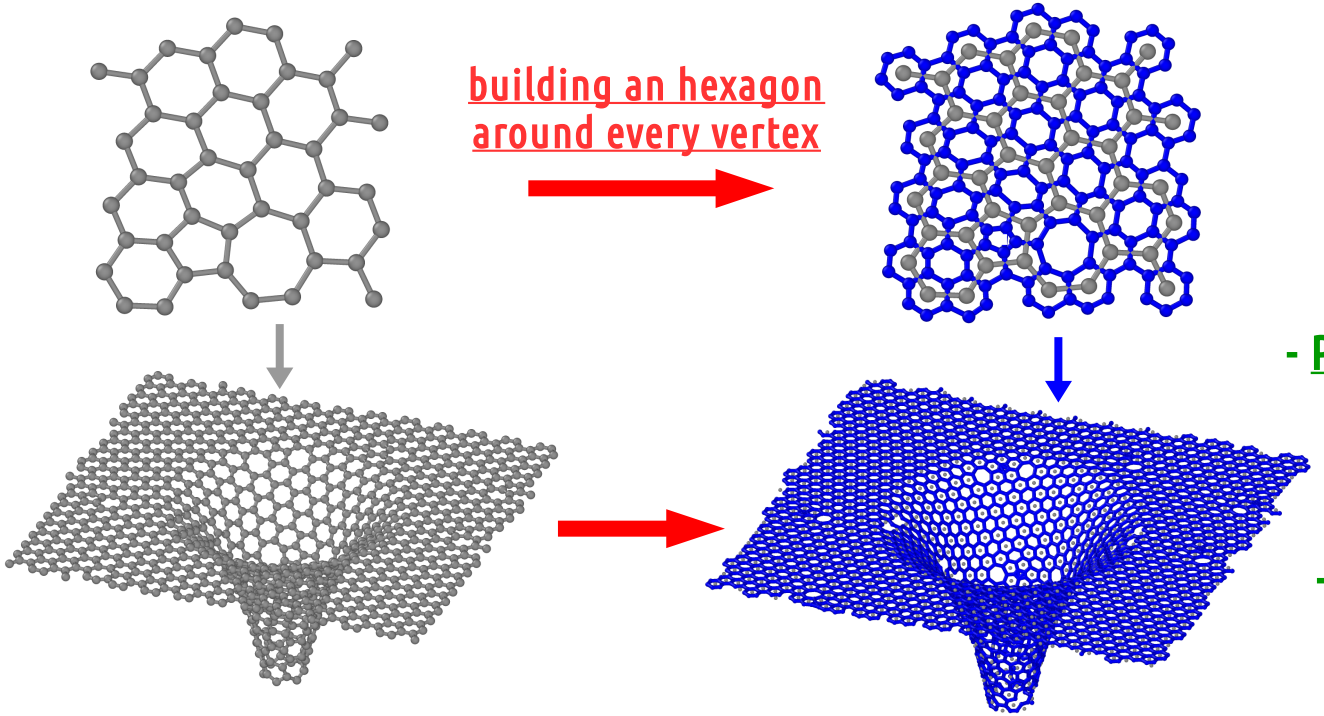
Theoretical reasons to increase the size: the model works for $|E|<\hbar v_F/R$

Numerical reasons to increase the size: high resolution of DOS around Fermi level

Idea: minimize a 'small' structure and increase dimensions with a *dualization algorithm*, exploiting the 3-coordination of the planar graph.

Local dualization

Global dualization



After stretching:

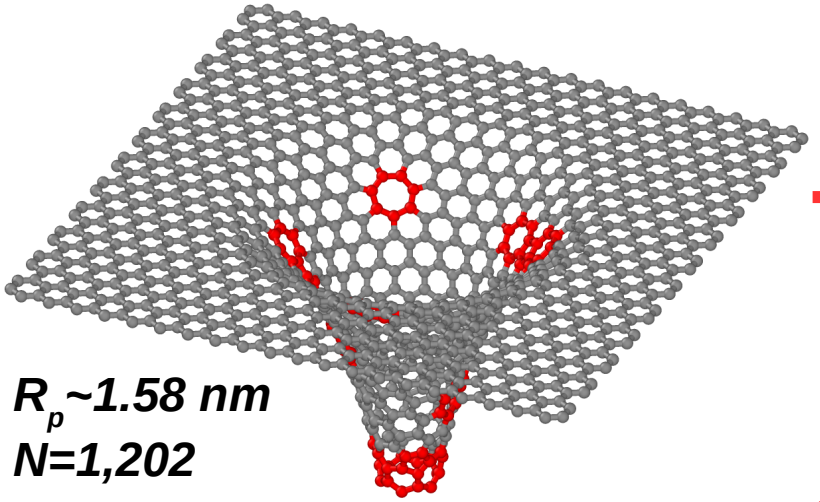
- Pseudosphere radius

$$R_{new} = \sqrt{3}\, R_{old}$$

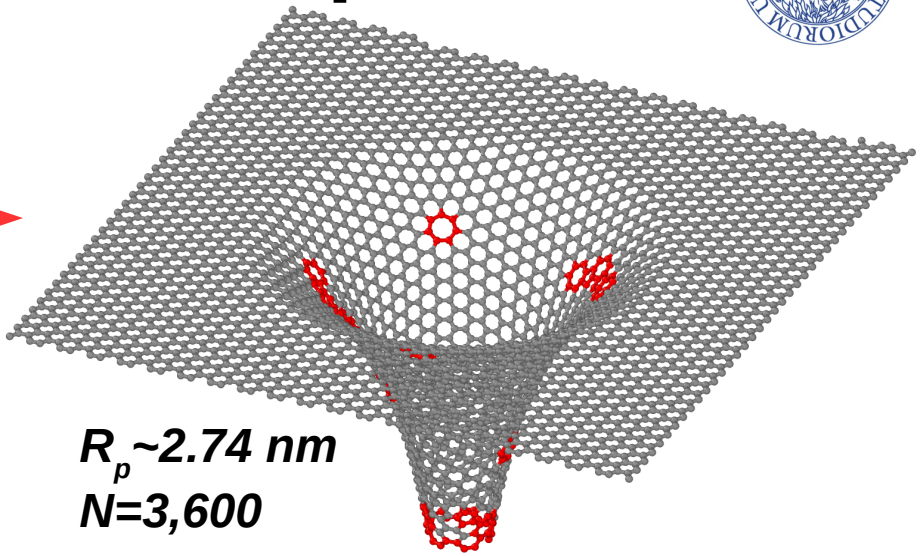
- Number of atoms

$$N_{new} \simeq 3\, N_{old}$$

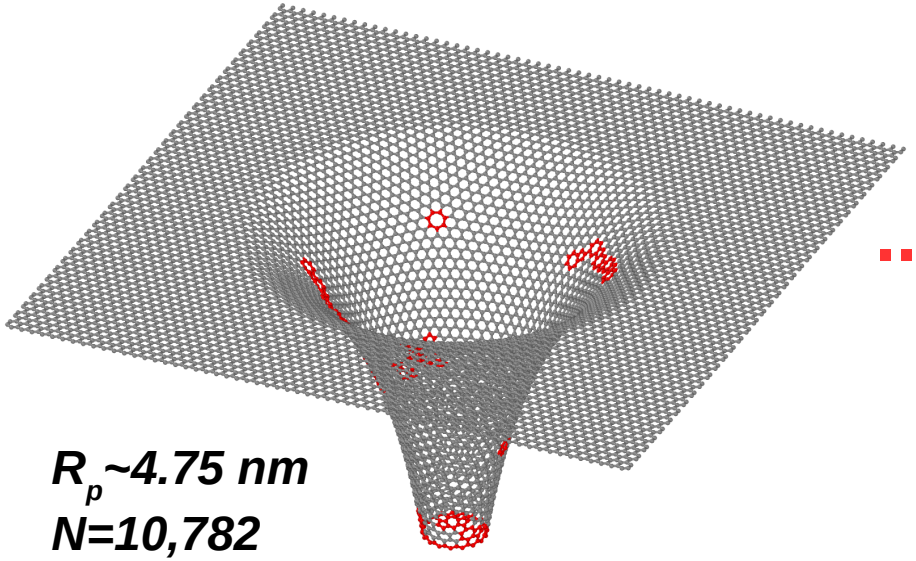
II. Building carbon pseudospheres



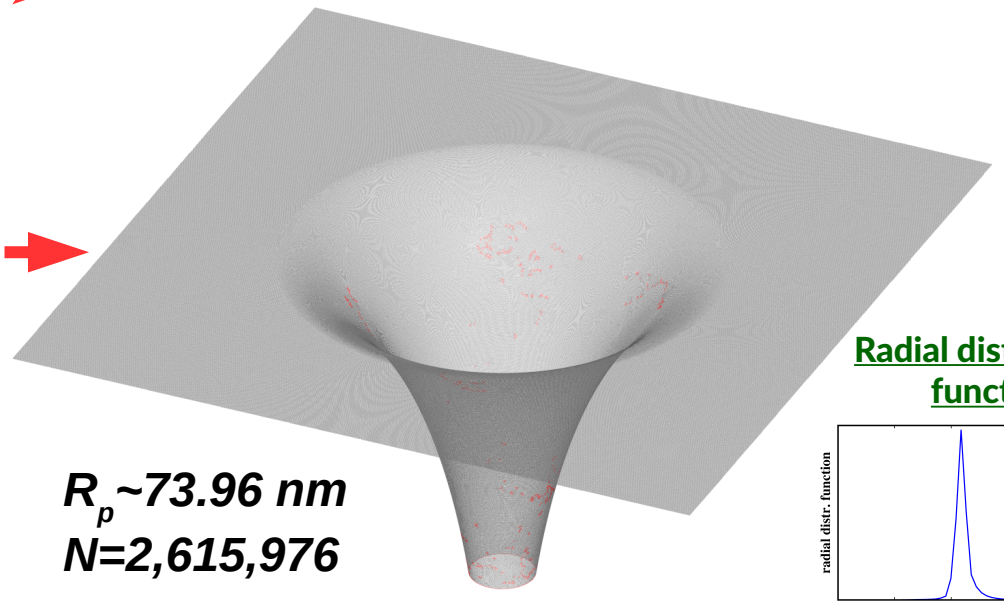
R_p~1.58 nm
N=1,202



R_p~2.74 nm
N=3,600

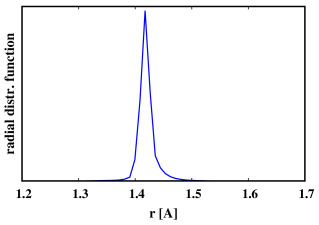


R_p~4.75 nm
N=10,782



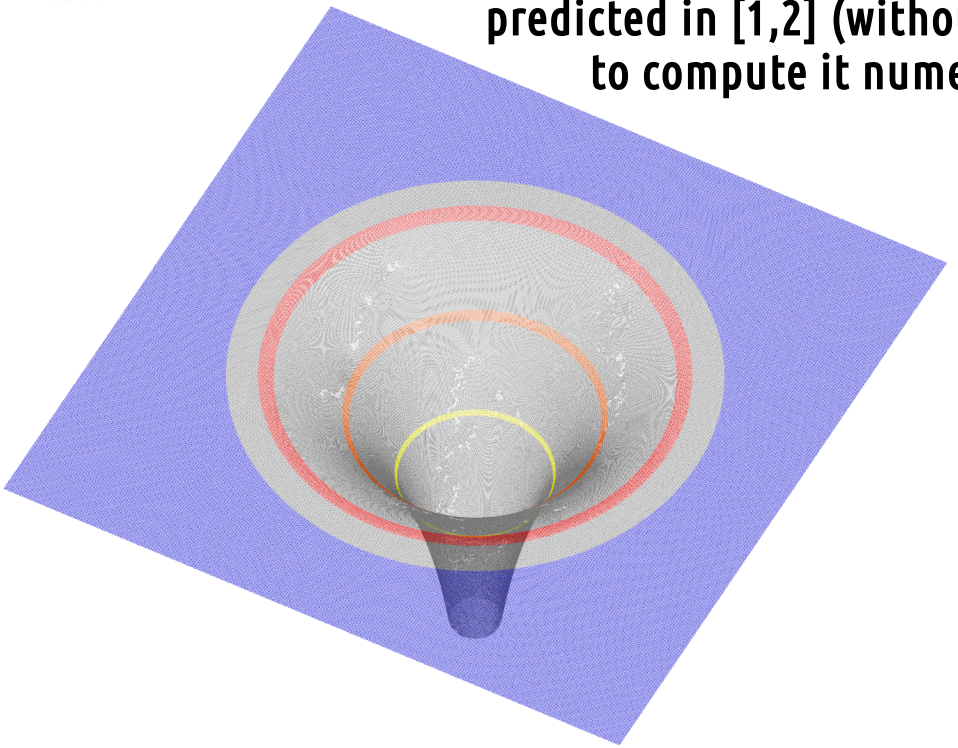
R_p~73.96 nm
N=2,615,976

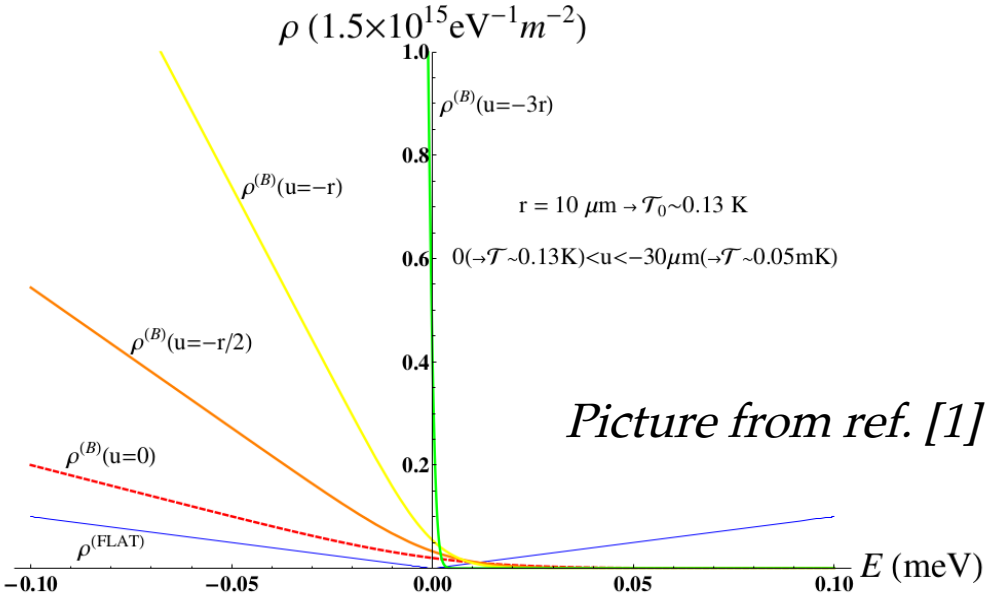
Radial distribution function



III. Electronic structure simulations

This is the behavior for the Local Density of States (LDOS) predicted in [1,2] (without boundary conditions [2]). How to compute it numerically in such big systems?





Picture from ref. [1]

Numerically: *kernel polynomial method* [7], which is based on Chebyshev expansion algorithms and it is ideal for a *tight binding approximation* (easiest approach).

$$\hat{H}=\sum_{\xi,i}\epsilon^{i}_{\xi}a^{\dagger}_{i,\xi}a_{i,\xi}+\sum_{\xi,\gamma,\langle ij\rangle}t^{ij}_{\xi,\gamma}a^{\dagger}_{i,\xi}a_{j,\gamma}$$

[1] A. Iorio, G. Lambiase, *The Hawking-Unruh phenomenon on graphene*, Phys. Let. B 716 (2), September 2012

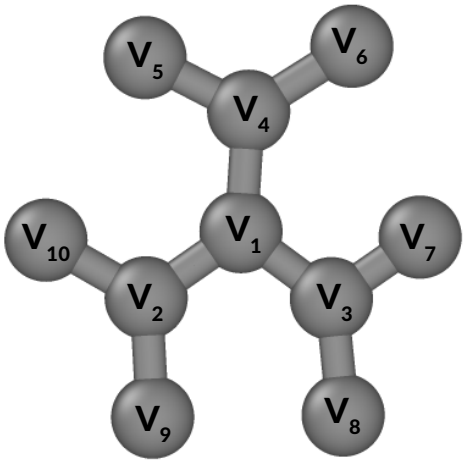
[2] A. Iorio, G. Lambiase, *Quantum field theory in curved graphene spacetimes, Lobachevsky geometry, Weyl symmetry, Hawking effect, and all that*, Phys. Rev. D 90, 025006, July 2014

[7] A. Weiße et al., *The kernel polynomial method*, Rev. Mod. Phys. 78, January 2006

III. Electronic structure simulations

A sketch of the tight binding Hamiltonian matrix within the nearest neighbor approximation

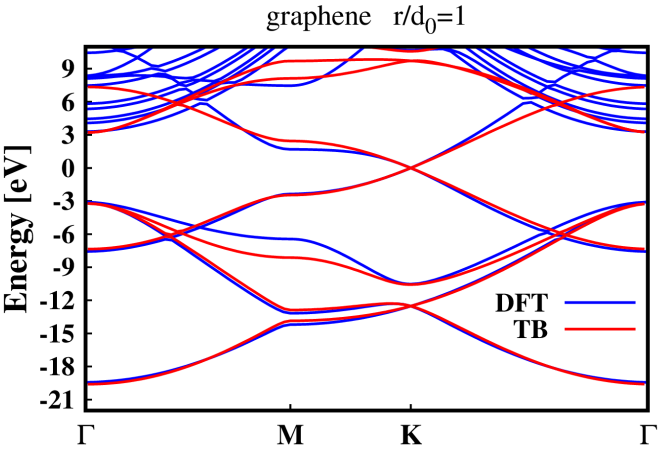
$$\begin{pmatrix}
I^{V_1} & M^{V_1,V_2} & M^{V_1,V_3} & M^{V_1,V_4} & 0 & 0 & 0 & 0 & 0 & 0 \\
M^{V_2,V_1} & I^{V_2} & 0 & 0 & 0 & 0 & 0 & 0 & M^{V_2,V_9} & M^{V_2,V_{10}} \\
M^{V_3,V_1} & 0 & I^{V_3} & 0 & 0 & 0 & M^{V_3,V_7} & M^{V_3,V_8} & 0 & 0 \\
M^{V_4,V_1} & 0 & 0 & I^{V_4} & M^{V_4,V_5} & M^{V_4,V_6} & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & M^{V_5,V_4} & I^{V_5} & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & M^{V_6,V_4} & 0 & I^{V_6} & 0 & 0 & 0 & 0 \\
0 & 0 & M^{V_7,V_3} & 0 & 0 & 0 & I^{V_7} & 0 & 0 & 0 \\
0 & 0 & M^{V_8,V_3} & 0 & 0 & 0 & 0 & I^{V_8} & 0 & 0 \\
0 & M^{V_9,V_2} & 0 & 0 & 0 & 0 & 0 & 0 & I^{V_9} & 0 \\
0 & M^{V_{10},V_2} & 0 & 0 & 0 & 0 & 0 & 0 & 0 & I^{V_{10}}
\end{pmatrix}$$



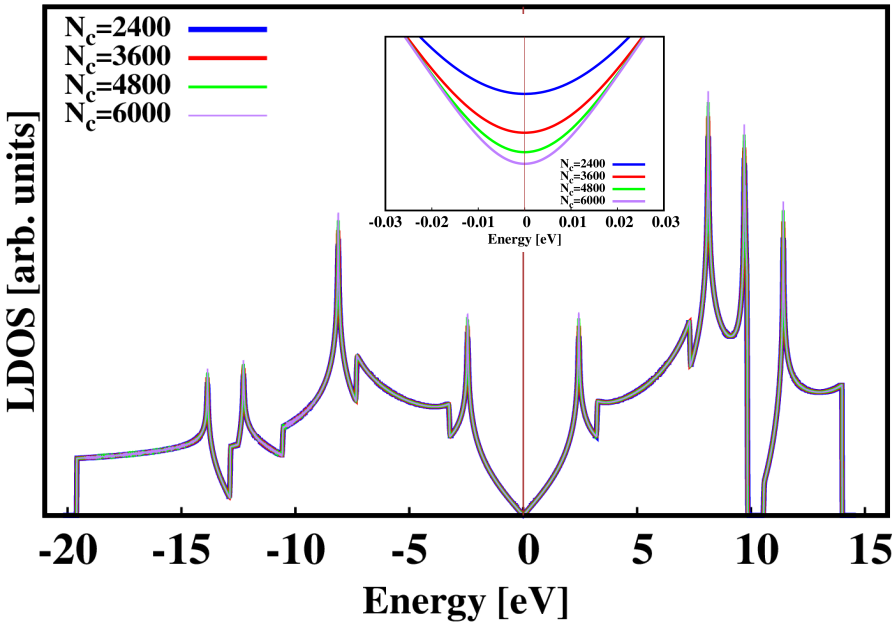
where $M^{i,j} = \begin{pmatrix} H^{i,j}_{s,s} & H^{i,j}_{s,p_1} & H^{i,j}_{s,p_2} & H^{i,j}_{s,p_3} \\ H^{i,j}_{p_1,s} & H^{i,j}_{p_1,p_1} & H^{i,j}_{p_1,p_2} & H^{i,j}_{p_1,p_3} \\ H^{i,j}_{p_2,s} & H^{i,j}_{p_2,p_1} & H^{i,j}_{p_2,p_2} & H^{i,j}_{p_3,p_2} \\ H^{i,j}_{p_3,s} & H^{i,j}_{p_3,p_1} & H^{i,j}_{p_3,p_2} & H^{i,j}_{p_3,p_3} \end{pmatrix}$ **and** $I^{i} = \begin{pmatrix} E^{i}_{s} & 0 & 0 & 0 \\ 0 & E^{i}_{p_1} & 0 & 0 \\ 0 & 0 & E^{i}_{p_2} & 0 \\ 0 & 0 & 0 & E^{i}_{p_3} \end{pmatrix}$

While on flat graphene only one p_z orbital per atom is sufficient to investigate low energy excitations, here all the 4 valence orbitals of carbon atoms are necessary to take into account the different overlap between atoms sitting on a curved surface.

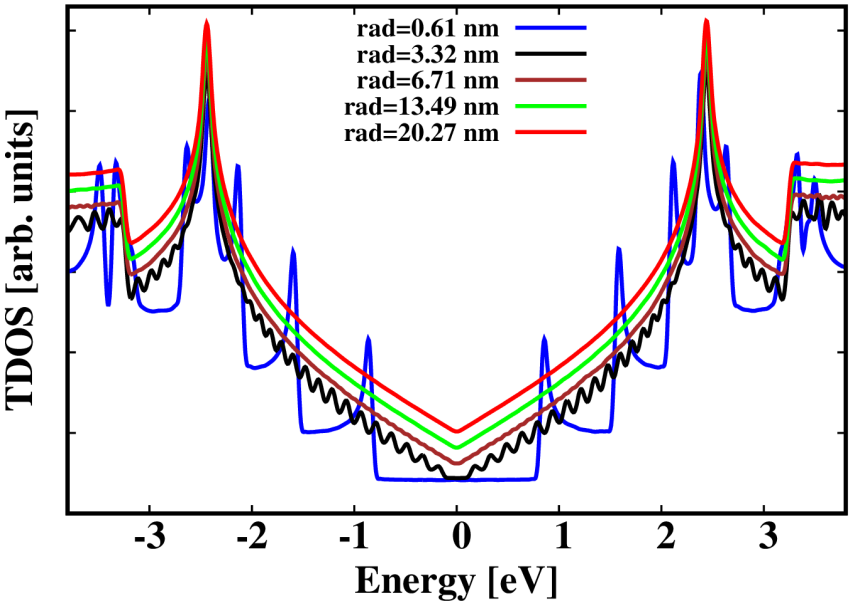
For the matrix elements we fit DFT calculations, obtaining accurate values for TB parameters



III. Electronic structure simulations



Tests of the electronic DOS code: two well known systems such as planar graphene and (n,n) carbon nanotubes



In general, a function f(x): [-1,1] → ℝ can be expanded as

$$f_{KPM}(x)=\frac{1}{\pi\sqrt{1-x^2}}\left[g_0\mu_0+2\sum_{n=1}^{\infty}g_n\mu_n T_n(x)\right]$$

where $\mu_n=\int_{-1}^{1} f(x)T_n(x)\,dx$

In our case, DOS:

$$\rho(E)=\frac{1}{D}\sum_{k=0}^{D-1}\delta(E-E_k)$$

I Chebyshev polynomial

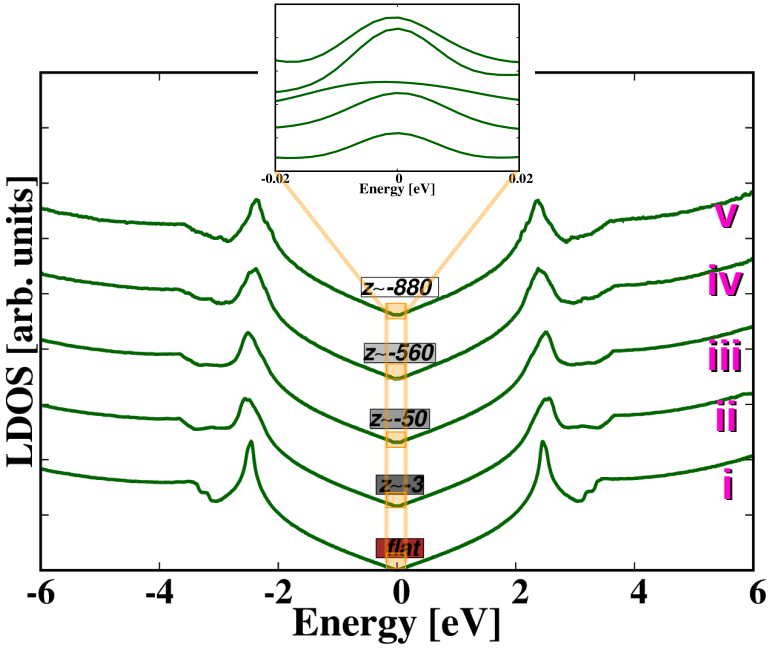
$$T_n(x)=\cos\left[n\cdot acos(x)\right]$$

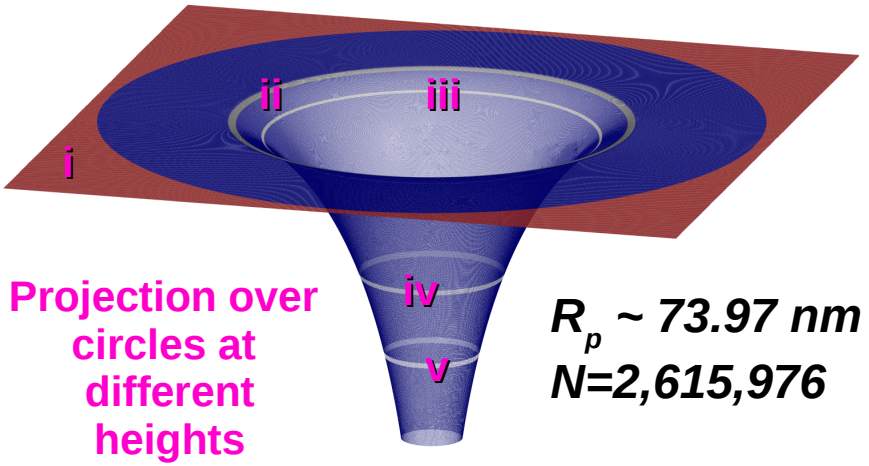
I Chebyshev polynomial recurrence relations

$$T_0(x)=1;\ T_{-1}(x)=T_1(x)=x$$
$$T_{m+1}(x)=2x\,T_m(x)-T_{m-1}(x)$$

III. Electronic structure simulations

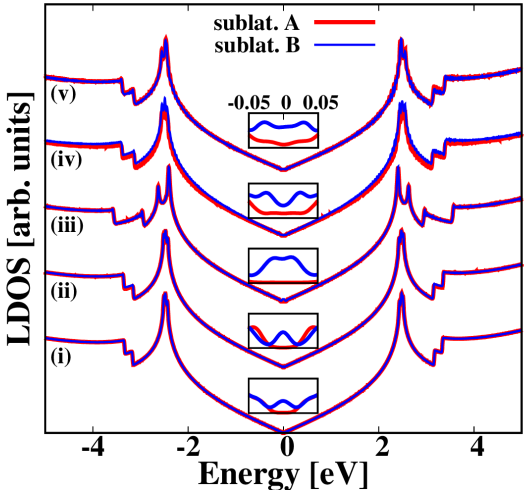
We perform different kind of analysis of the Density Of States

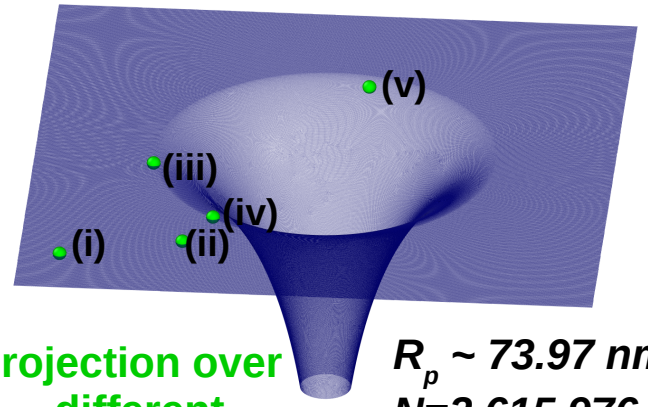




Projection over circles at different heights

R_p ~ 73.97 nm
N=2,615,976

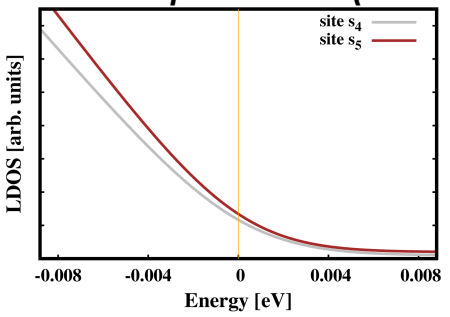




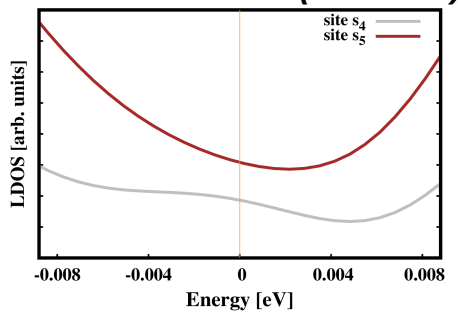
Projection over different atomic sites

R_p ~ 73.97 nm
N=2,615,976

Theoretical predictions (Iorio et al.)



Numerical results (this work)



Here we take some atomic sites and we compare the results with the theoretical predictions

IV. Conclusions

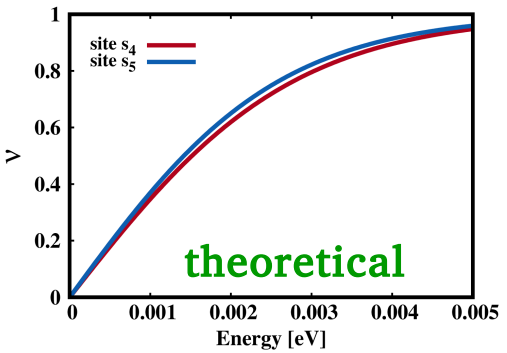
- The methods used can be exploited to model graphene-like structure on different and more complex surfaces. The algorithm adopted to scale up with dimensions could be useful also for other multi-scale modeling problems in, at least, sp^2 structures;
- **Tight binding approach used in conjunction with Kernel Polynomial Method can give useful insights at low computational cost for the electronic properties.**

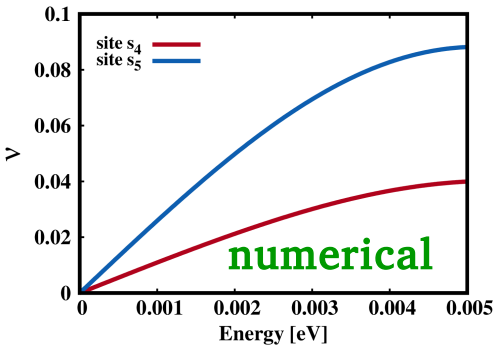
Can our model confirm the predictions of [1,2]?

We found an asymmetric behavior of the LDOS.
This finding comes from the presence of heptagonal and pentagonal defects in the structure that must be present due to the negative Gaussian curvature (Gauss-Bonnet theorem).

However it is difficult to compare our results with the ones of [1,2].

v measures the asymmetry of the LDOS





Our model includes elastic effects and the broken translational symmetry of graphene lattice (A and B sublattices) plays an important role.

T. Morresi et al., *arXiv:1907.08960* (available from 24 July 2019)

The other members behind this work

- **S. Taioli**

- **N. M. Pugno**

- **D. Binosi**

- **S. Roche***

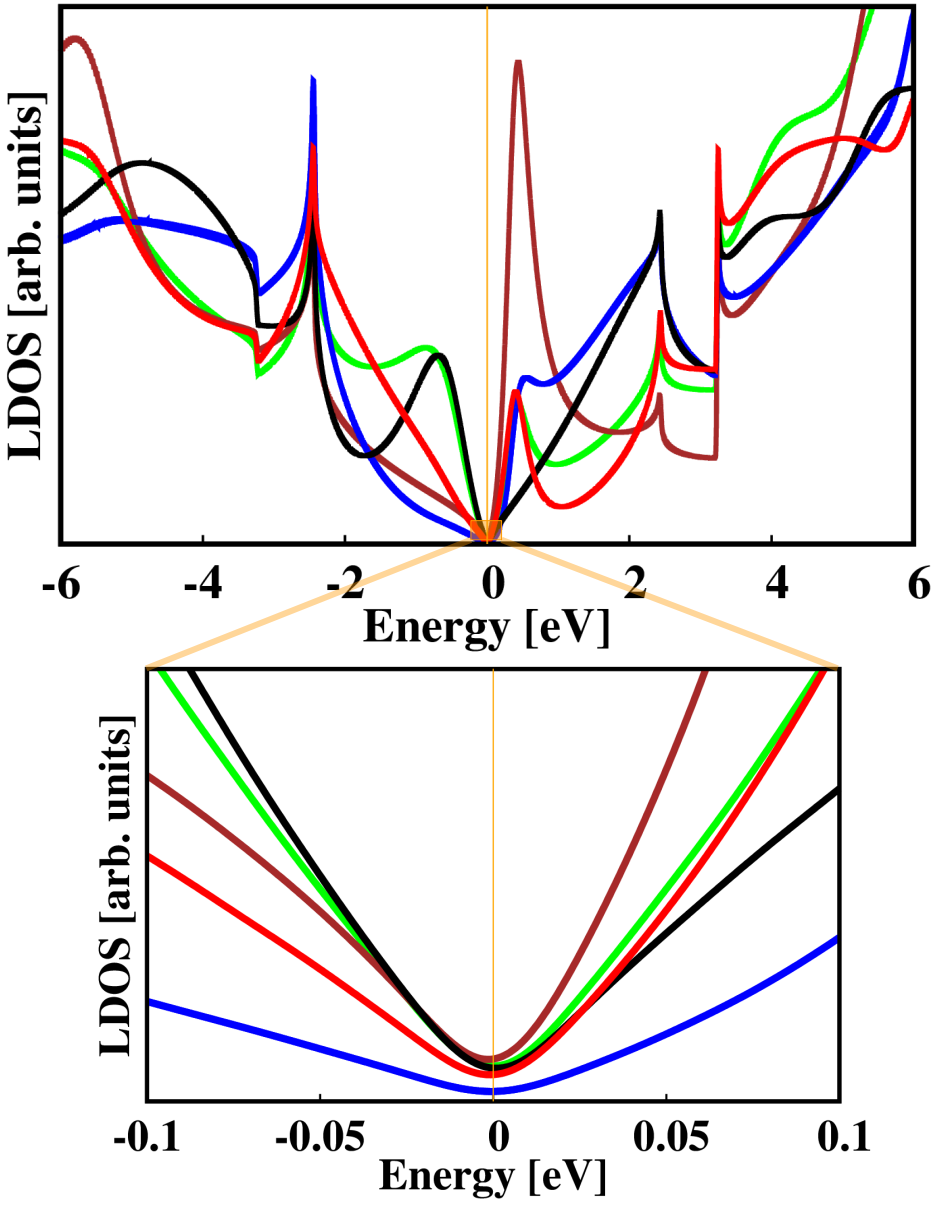
- **S. Simonucci****

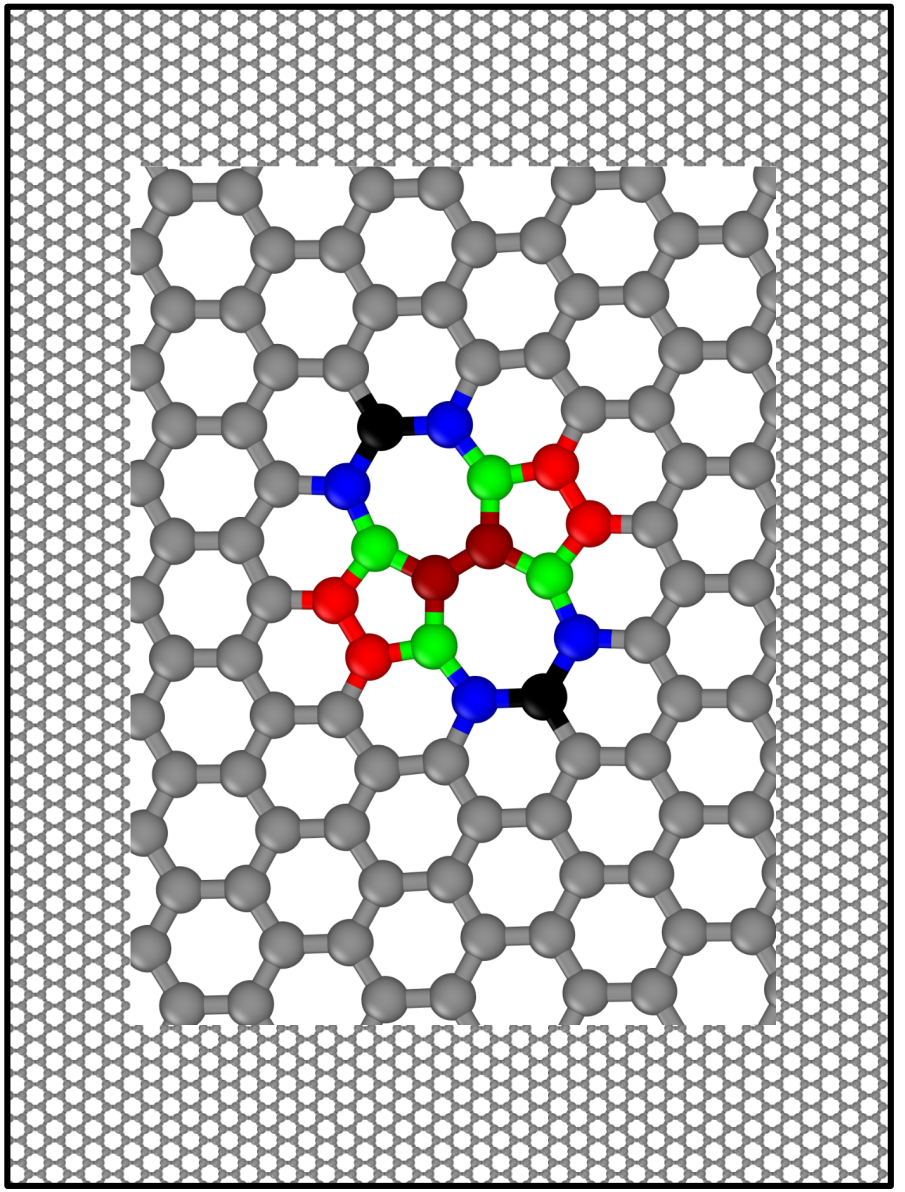
- **R. Piergallini****

[*] *Catalan Institute of Nanoscience and Nanotechnology, ICN2*, Barcelona, Spain
[**] *School of Science and Technology, University of Camerino,* Camerino, Italy

Thanks for the attention

Angular dependence LDOS due to a Stone-wales defect





Radial dependence LDOS due to a Stone-wales defect