In silico optimization of tritiated graphene for Ptolemy

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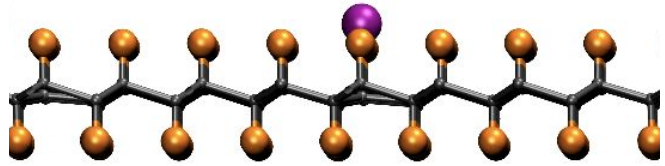
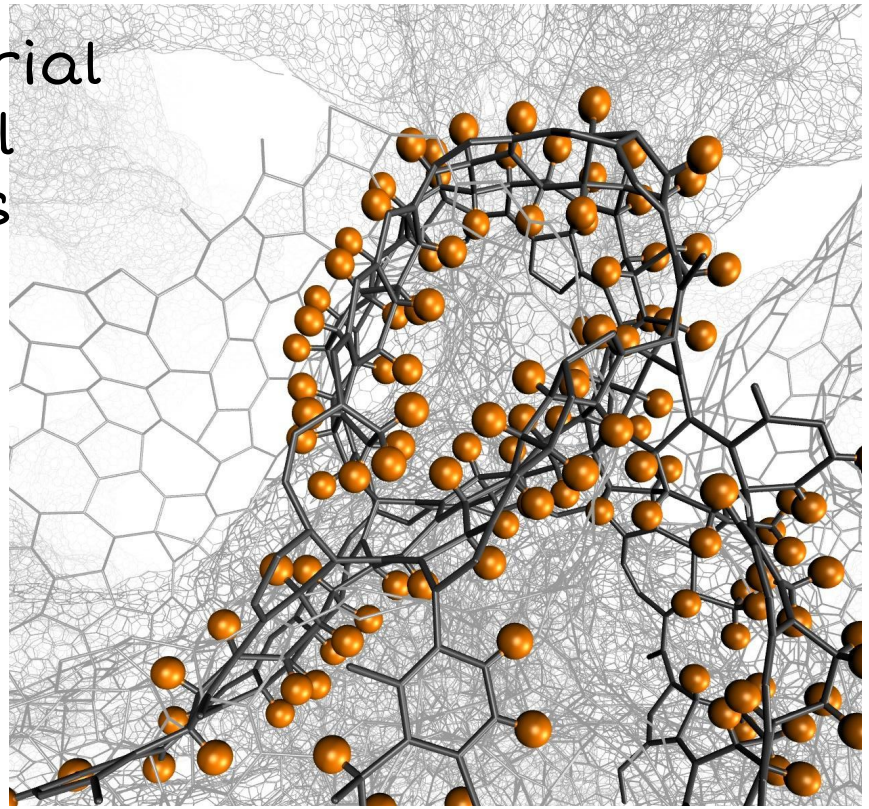
PTOLEMY collaboration

Outline

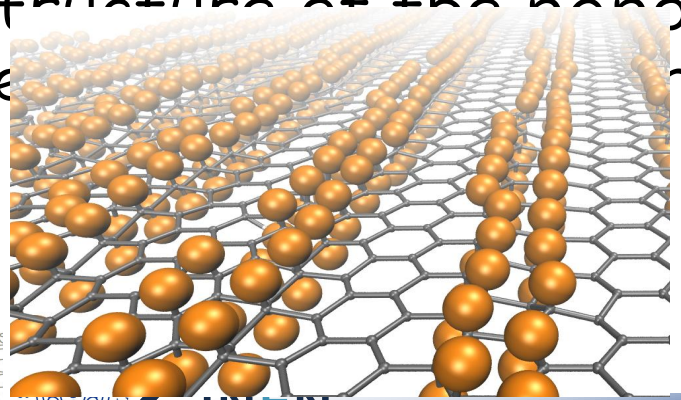
- ✔ What happens *during* 3H decay
  - Potential of tritium on graphene → quantum uncertainty corrections

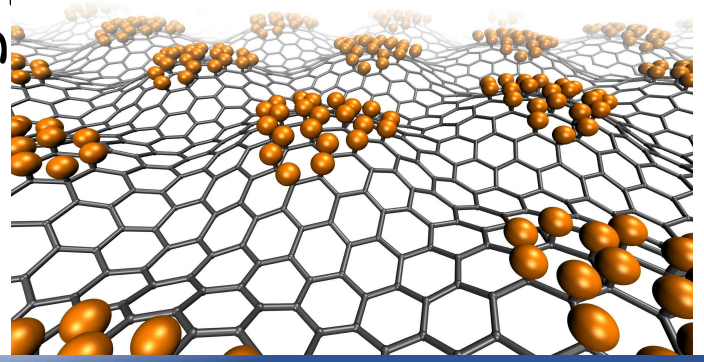


- ✔ What happens *after* decay(/capture)
  - Electronic structure relaxation
  - He dynamics and interaction with the material
  - Interaction of β electrons with the material
    → Energy loss function & MC simulations



- ✔ How do we optimize the material?
  - Structure of the nanoporous scaffold
  - Le[illegible]n



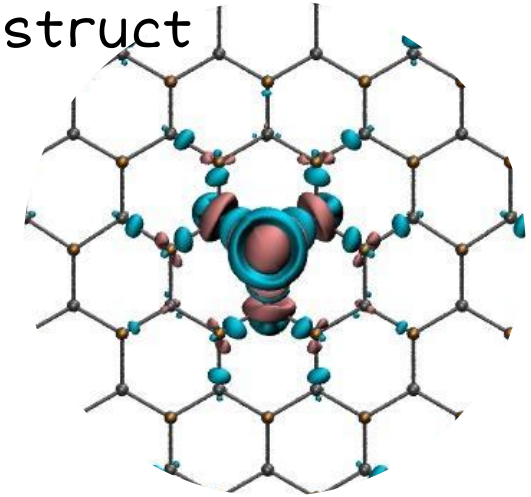


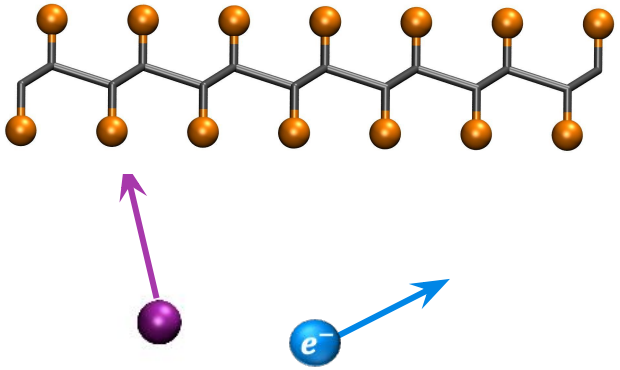
Timeline

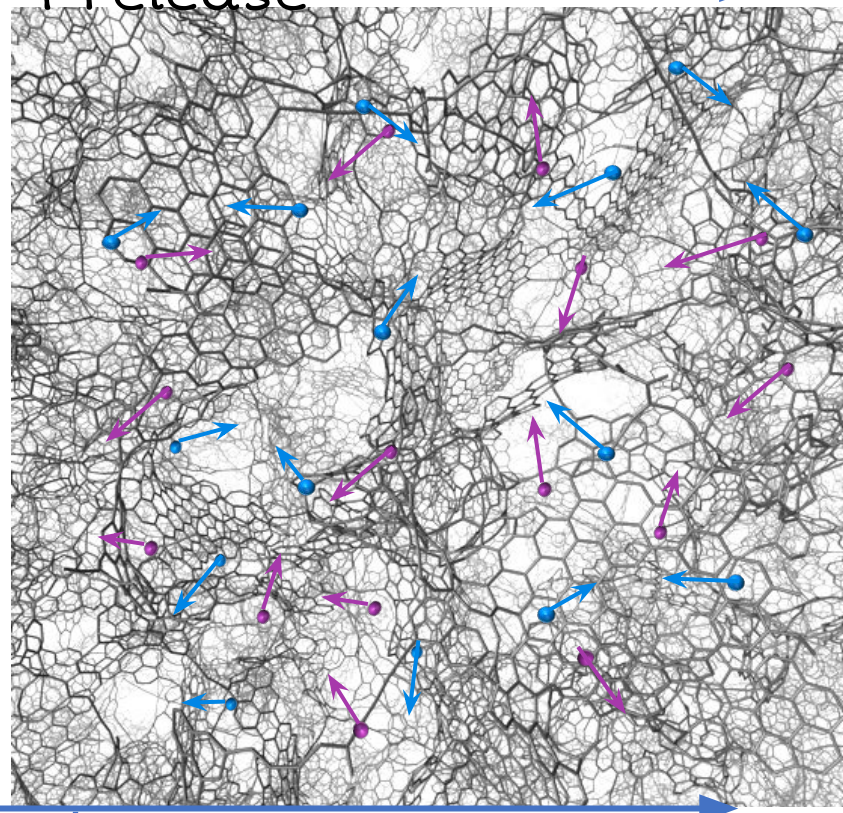
Electronic relaxation from 3H to He el struct

He detachment

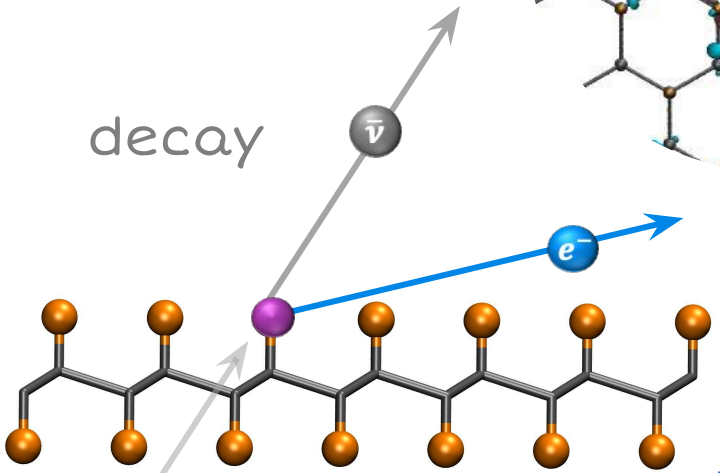
He and β diffusion & interaction
Heating up
Material damage
T release

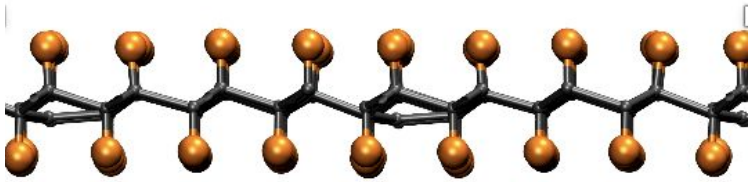






decay





t=0

t~fs-ps

t~ ns-μs

(captur
e)

On the ultra-fast time s

Electrons space density

$$E[n(\mathbf{r})](z) = E_{ee}[n(\mathbf{r})] + \int n(\mathbf{r}) V_{N,e}(\mathbf{r}, z)\, d\mathbf{r} + V_{NN}(z)$$

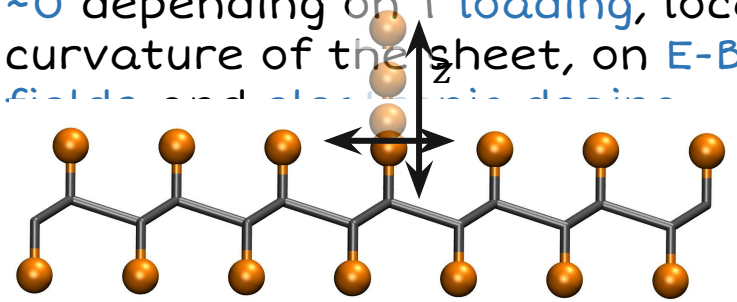
El-el interaction

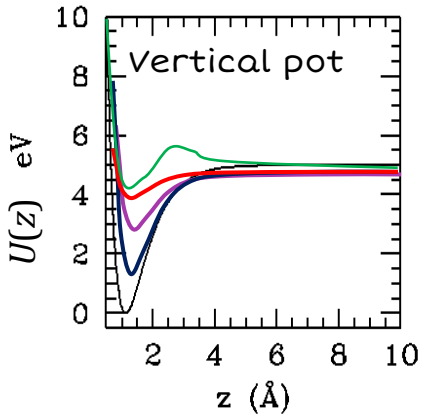
Nuclei-electron interaction

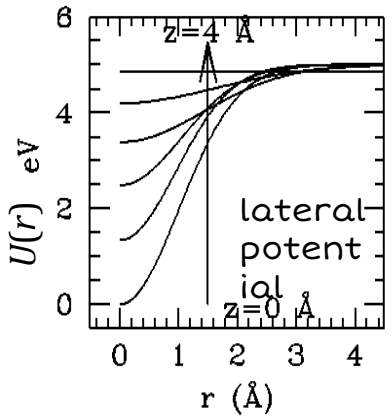
nuclei int

Before decay/capture:

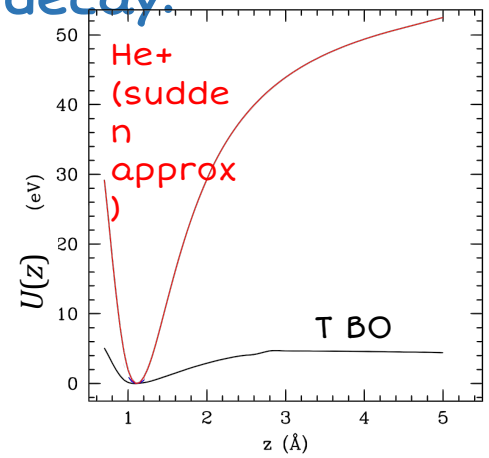
- ✔ $n(\mathbf{r})$ is relaxed in the electronic ground state
- ✔ The T interaction potential $U(z)$ is calculated within BO-DFT moving a T atom
- ✔ T binding energy ranges from 5 eV to ~0 depending on T loading, local curvature of the sheet, on E-B external fields and also on pic dosing

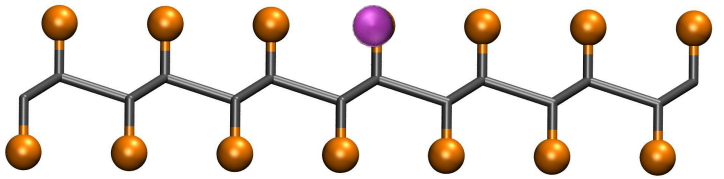




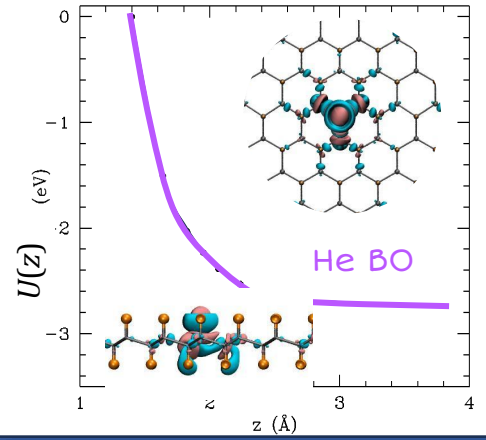


Just after decay:





- ✔ ^{3}H becomes He$^+$ and the electronic structure has not time to rearrange
- Sudden approximation : U(z) evaluated with $n(\mathbf{r})$ frozen at the configuration with T
- The potential is strongly attractive

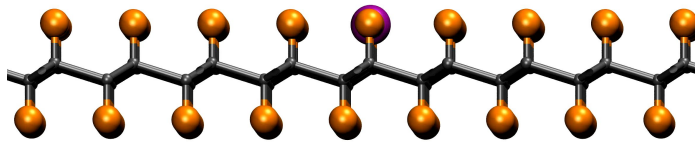


After electronic relaxation:

- ✔ Electrons move to He (He$^+$ → He)
- ✔ The potential turns strongly repulsive

The relaxation time depends on the opto-electronic properties of the material, and therefore on the T loading

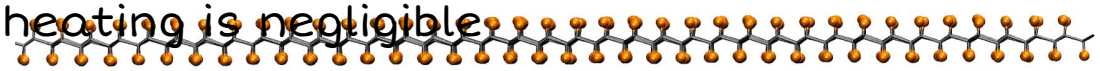
The repulsive potential produces He release

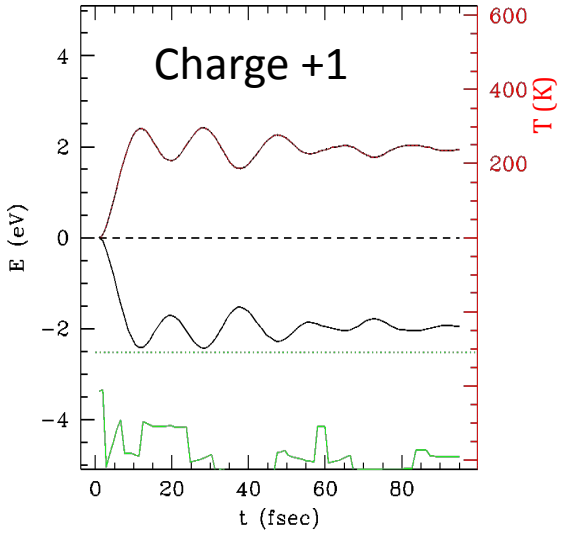


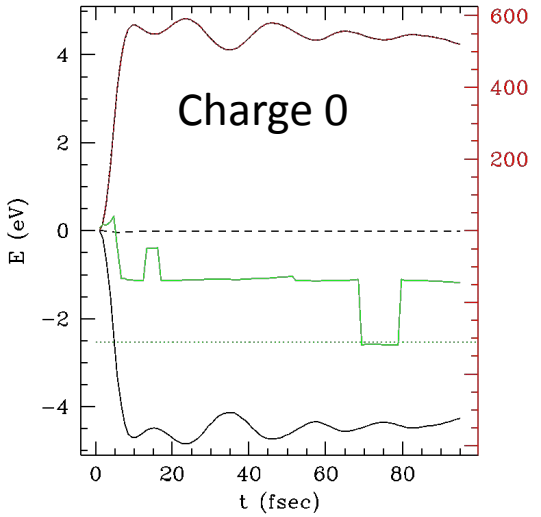
For each He released, **the system gains**

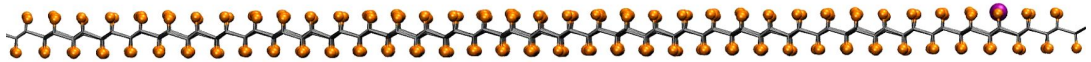
- ~2 eV if isolated (ch +1)
- ~4 eV if neutralized

He transfer energy to the sytem during ~10-100 ns.
A single event can heat locally (~1nm^2) up to 600K but given the low rate of events on the large scale heating is negligible

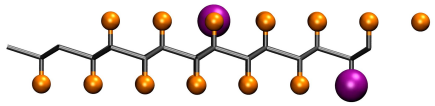


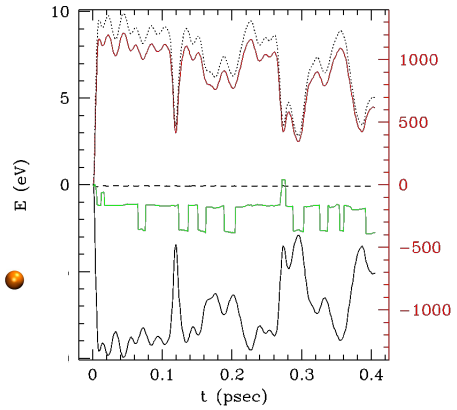


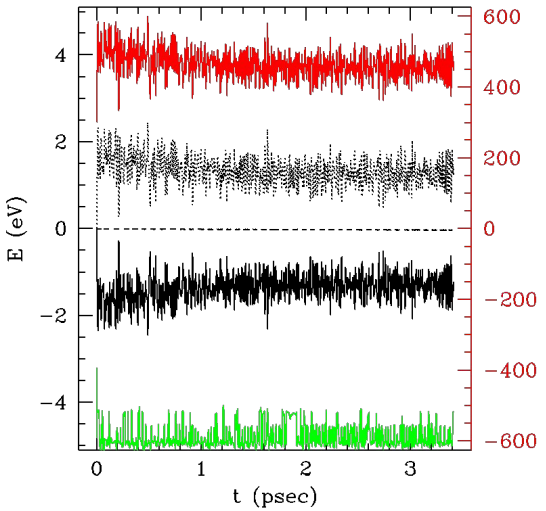


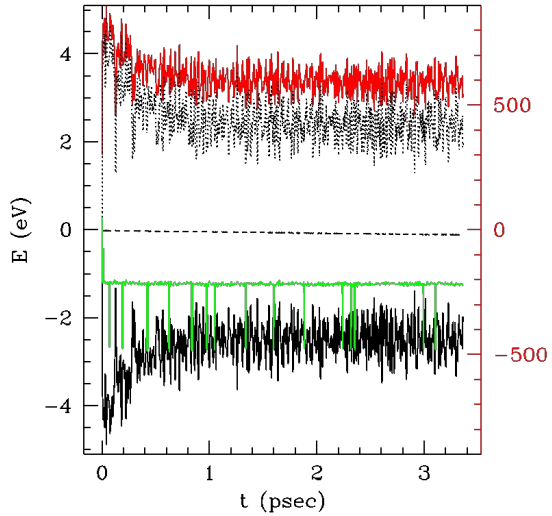


Double decay/release events (extremely unlikely) could have sufficient energy to create a vancancy in the sheet







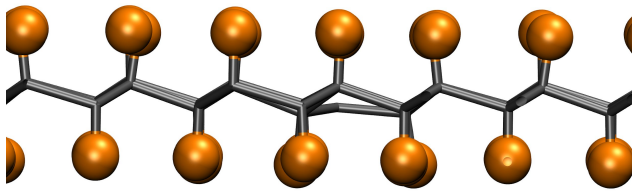


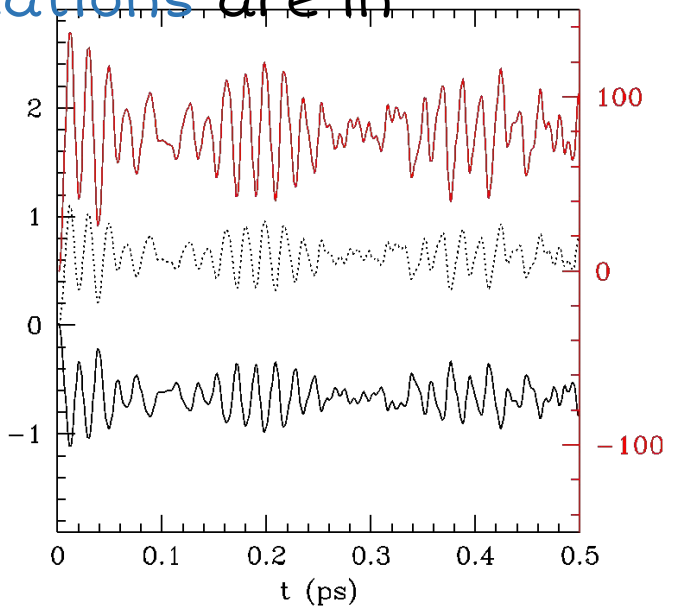
Overall, it seems that He release would not make substantial damage to the system

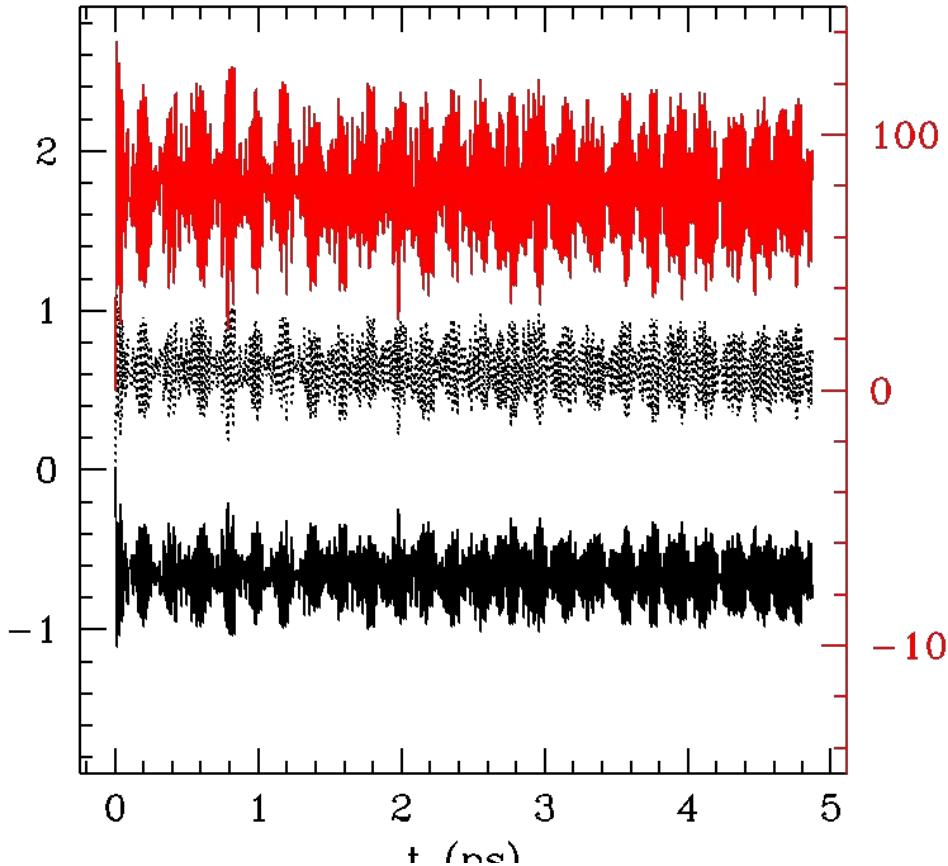
The He release excites specific modes of the sheet

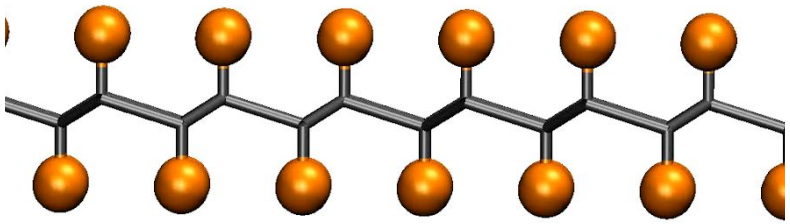
- ✔ After He is released, **the vacant site is distorted** and its relaxation excite **specific vibrational modes**
- ✔ These are visible in the beats and involve: stretching-bending and rocking + out of plane mode of the sheet
- ✔ Specific frequencies may appear as **enhanced peaks in IR or Raman**
- ✔ The frequencies however, depends on the amount and distribution of tritium

- ✔ Vibrational spectra calculations are in

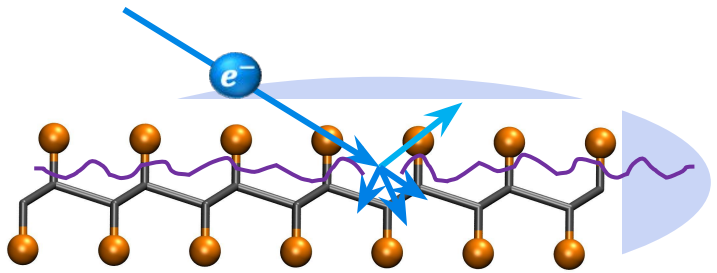








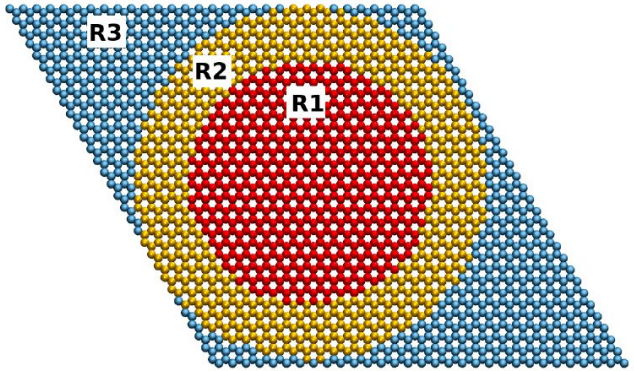
The β electrons interact with the material

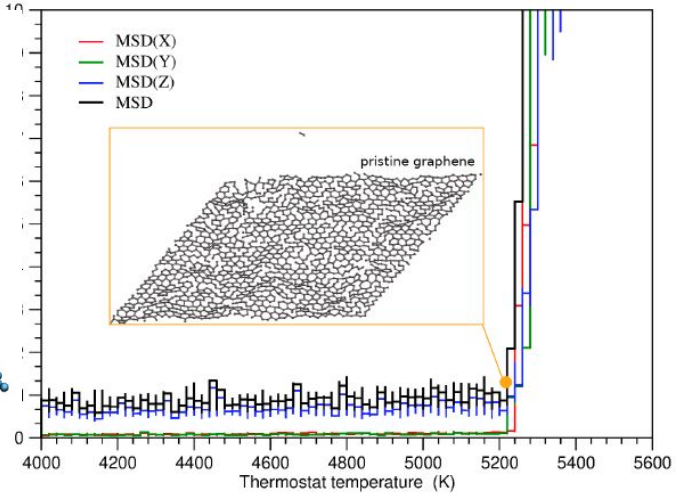


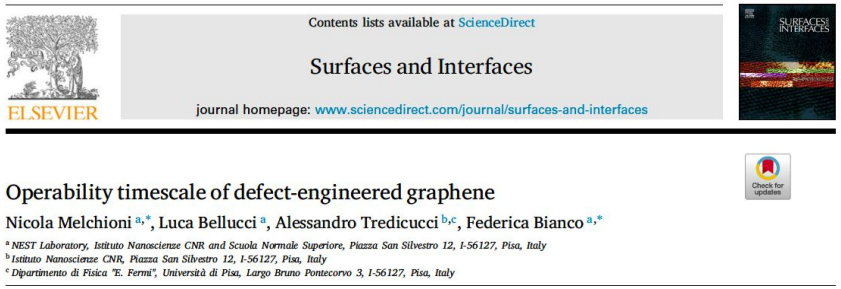
In the low energy range (up to 20-100K) electrons interact with the material and release energy with several mechanisms

- ✔ Primary scattering
- ✔ Production of secondaries and scattering
- ✔ Dissipation by interactions with electrons of the material
- ✔ Dissipation by interaction with phonons of the material

Moleculary dynamics simulations (L Bellucci) were previously done for **EMB electron beams (20keV) with very large fluence (5x10 ^{9} el/nm^{2} sec)** considering **only primary scattering** and other effects a producing an average gradual eating in the **local spot of the beam**



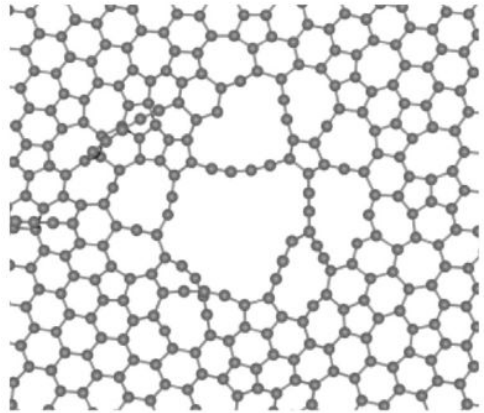




- ✔ The single scattering event can transfer to C ~3eV

⇒ **This cannot generally break C=C bonds**

- ✔ However, **the local heat up** of the sheet due to secondaries and dissipation can combine with the scattering and **create defects**



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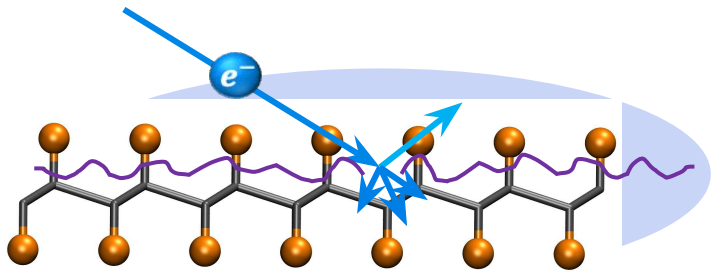

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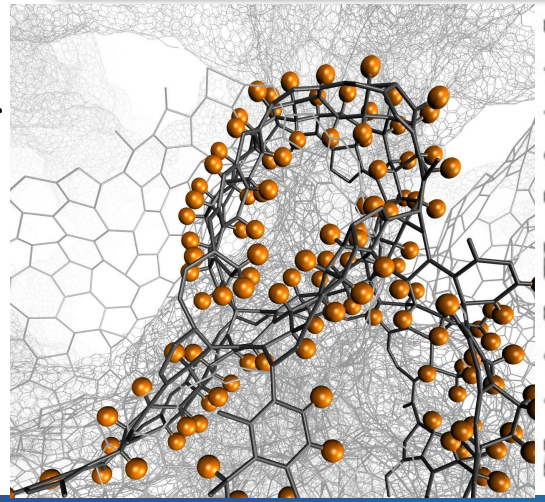
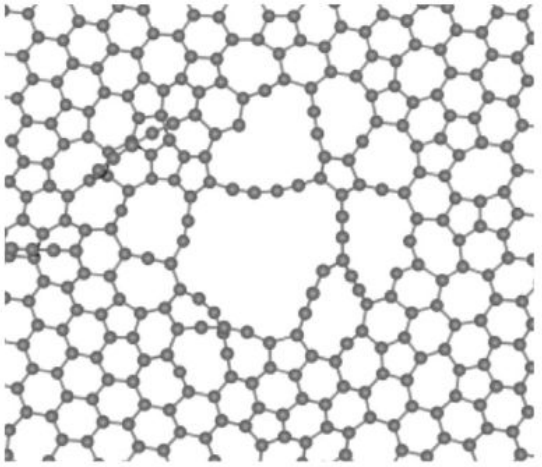
In our case

- ✔ The primary scattering can release up to **15 eV to ^{3}H** (due to smaller mass) and possibly **break C-H bond**
- ✔ On the other hand, we have much **lower fluence** (10^{-7} el/nm^2 sec) but we want to properly consider the distribution of secondaries and their scattering into the material
- ✔ Additionally, we have a **complex material** , both in composition and structure, and we must consider the dissipation both by electronic structure and phonons

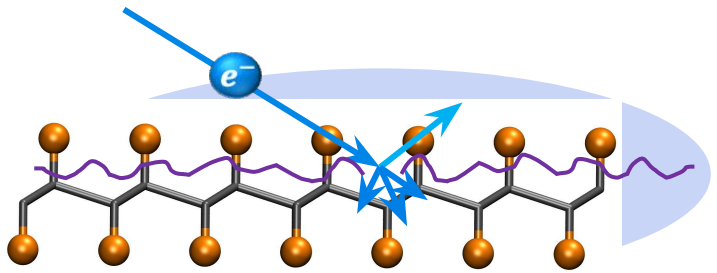
$$E_t = \left\{ 1 - \left(\frac{m_e \cos\omega' + \sqrt{m_c^2 - m_e^2 \sin^2\omega'}}{m_e + m_c} \right)^2 \right\} \frac{(E + 2m_e c^2)}{2m_e c^2} E, \quad (2)$$

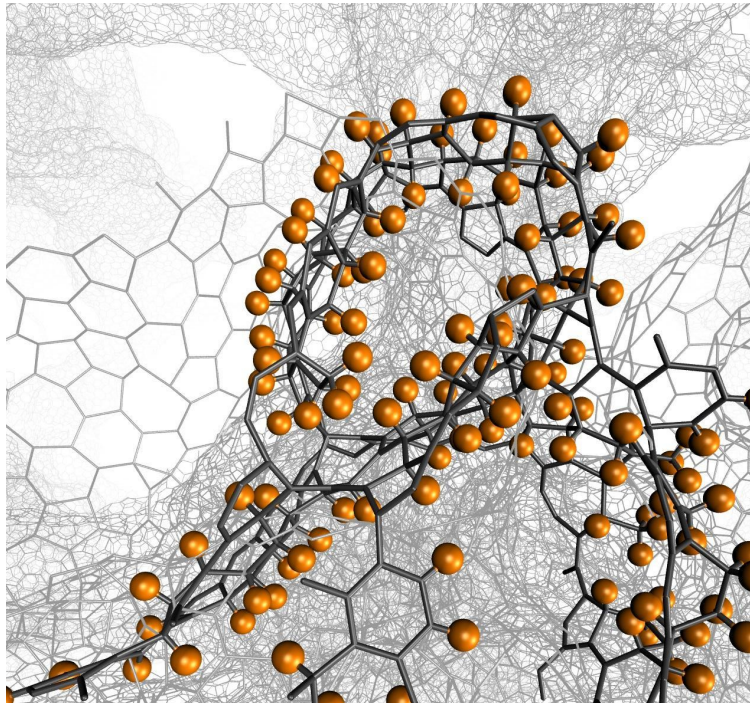
See e.g. Asayama et al, J Vac Sci Tech B 30 06fj02 2012





The β electrons interact with the material





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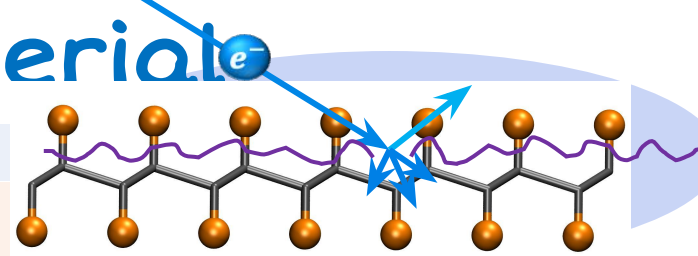
IDEA: combine **Monte Carlo (NEBULA)** with **MD**

- ✔ From MC simulation calculate the energy distribution in the structure
- ✔ Use that energy distribution to create the starting condition of in a structurally realistic model and evlove it with MD

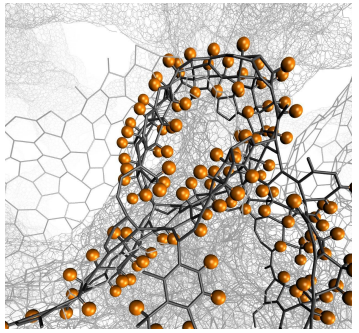
Issues:

- ✔ The effects to be described in MC simulations DEPEND on the material composition AND structure
- ✔ Tritiated graphene is **two dimensional, nano-porous** and **disordered**

The β electrons interact with the material



- ✔ Primary scattering — Chemical composition
- ✔ Production of secondaries and scattering — Electronic structure
- ✔ Dissipation by interactions with electrons of the material
- ✔ Dissipation by interaction with phonons of the material — Phonon dispersion



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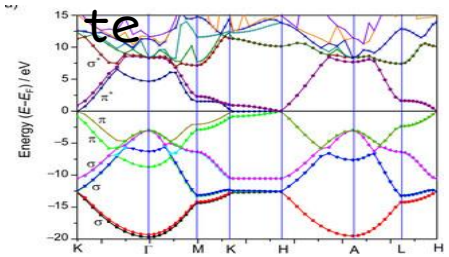
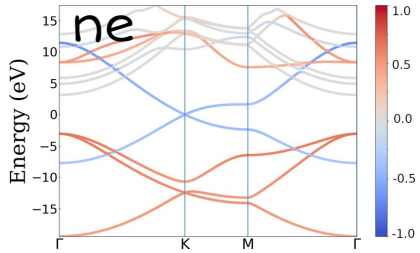
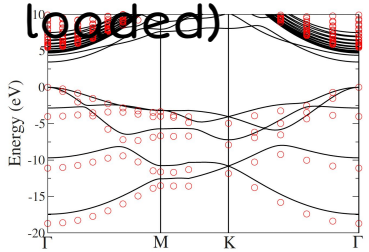
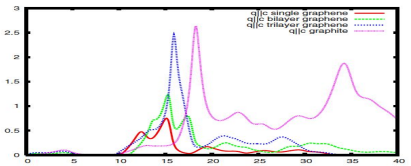
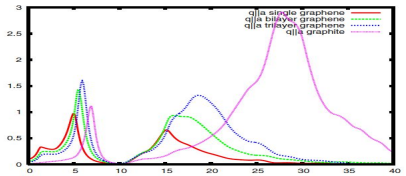
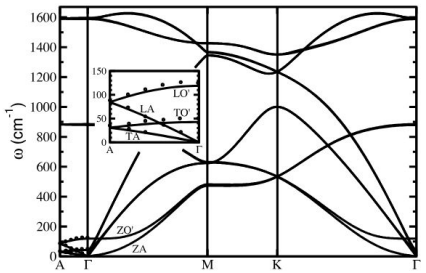
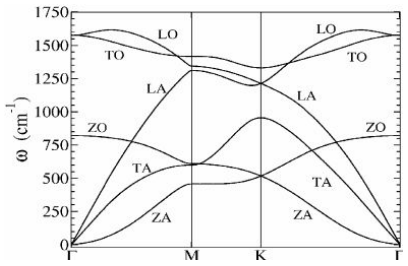
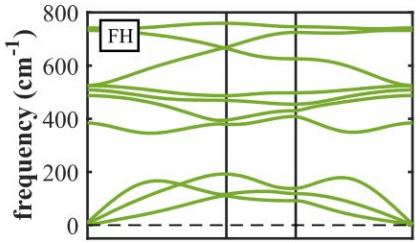
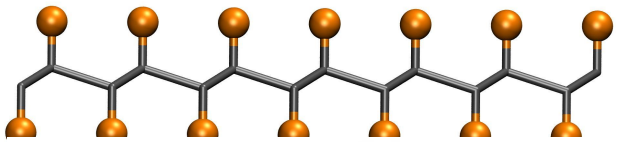
	Graphite	Graphene	GraphAne (fully loaded)
Electronic band structure			
Energy loss function/ conductivity			$\mathrm{Im}\left[\frac{-1}{\varepsilon(q,\omega)}\right]$
Phonons			

graphite : anisotropic conductor **graphene** : conductor 2D **graphAne** : insulator 2D

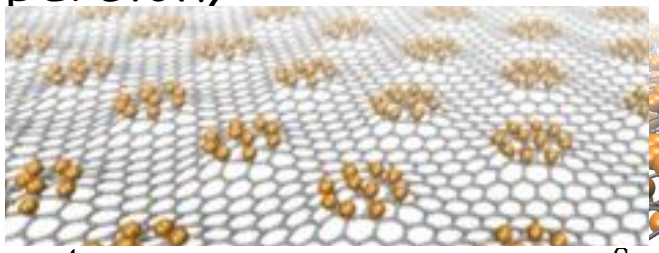
graphite : extremely anisotropic and dominated by plasmon peak **graphene/graphane** : 2D, and strongly dependent on momentum transfer

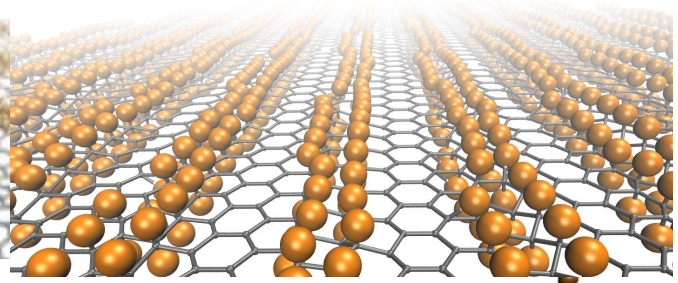
graphite : strongly anysotropic **graphene** : quadratic branch **graphAne** : quadratic branch and specific C-H optical modes

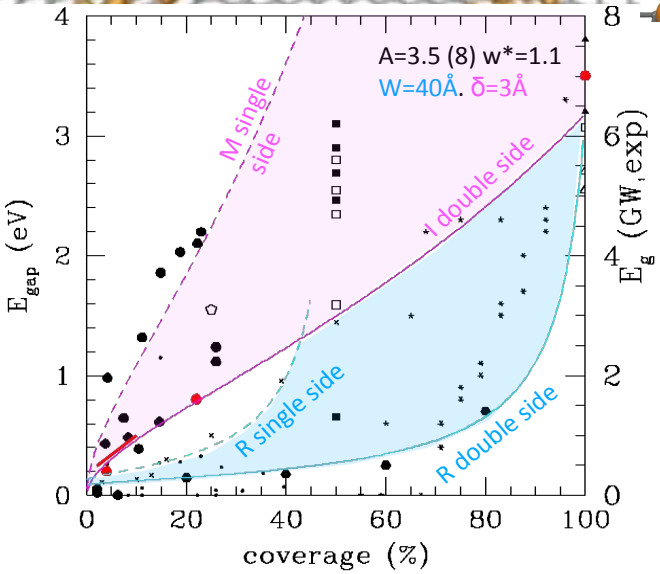
The "real" material and its properties

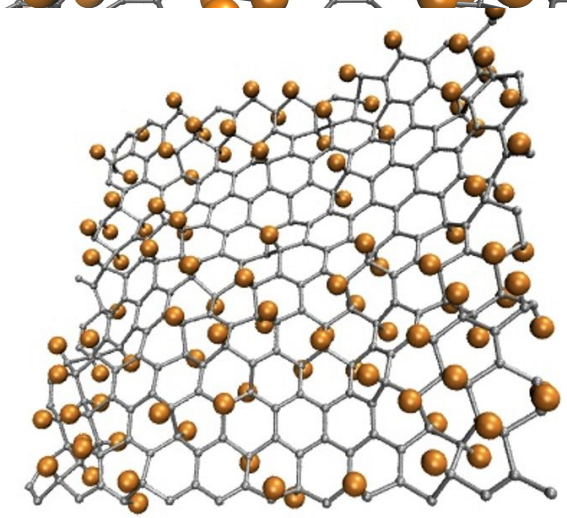


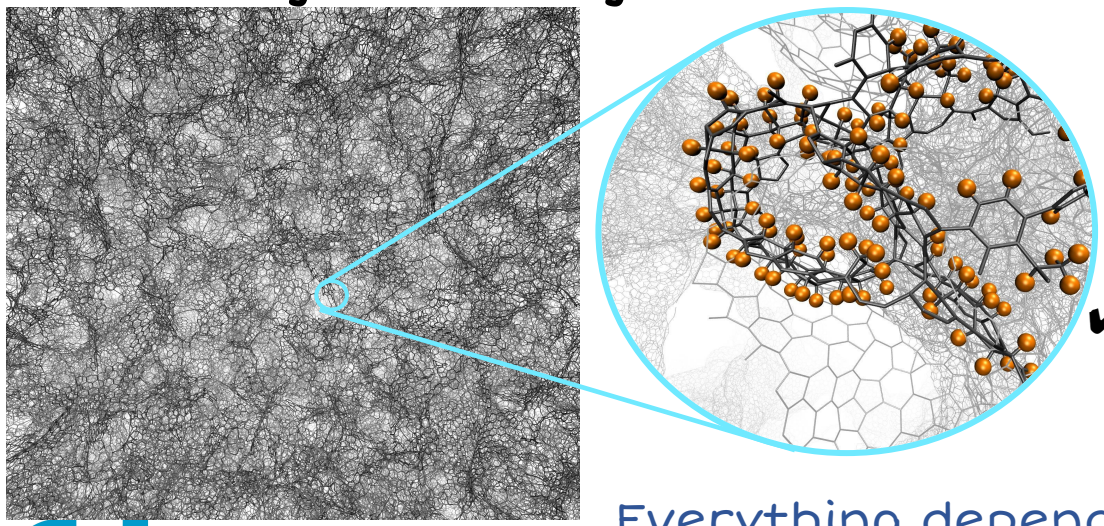
- ✔ Our material **is 2D** → Some of the properties are intrinsically different (density of states, phonons dispersion, conductivity, ELF)
- ✔ Our material is **not entirely graphene or graphAne**
- ✔ Our material is **not even regularly loaded**, but probably disordered
  → Properties like conductance, ELF, vibrational spectra are a mixture of those of graphene/graphAne, depending on **loading** and **configuration of tritium**









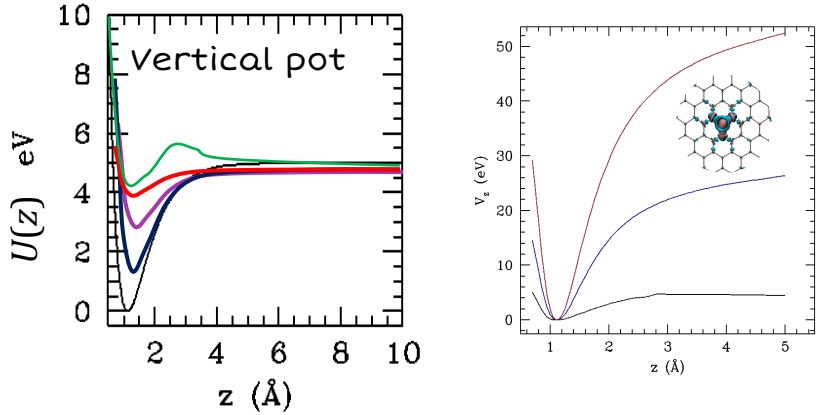


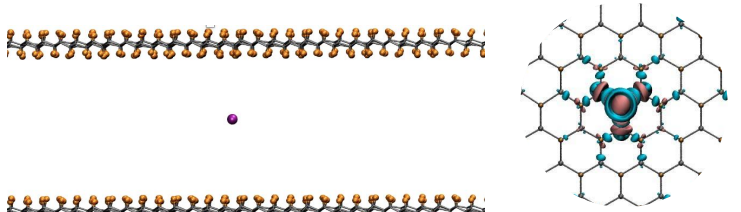
- ✔ Graphene is **nanoporous**
  → tritium loading, diffusion of He, β electrons interaction and vibrational properties are **influenced by the structure**

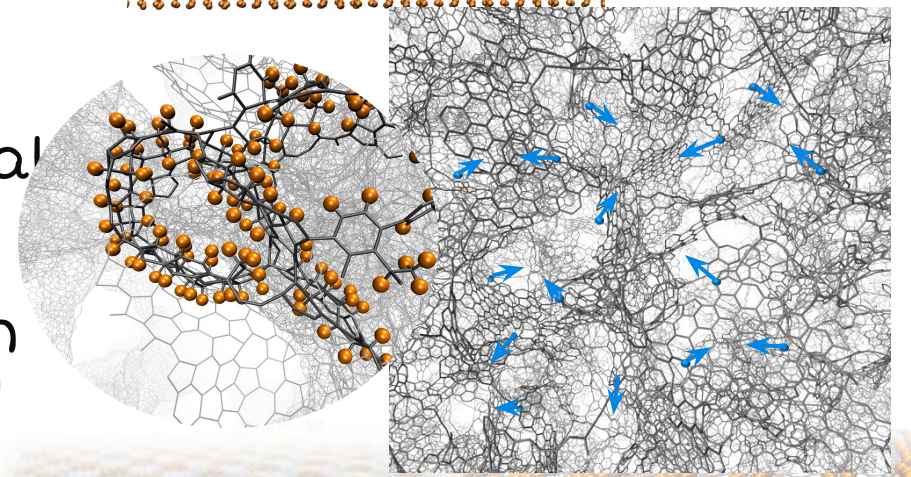
Everything depends on **graphene structure**, on **tritium loading** level and **distribution** !

Summary

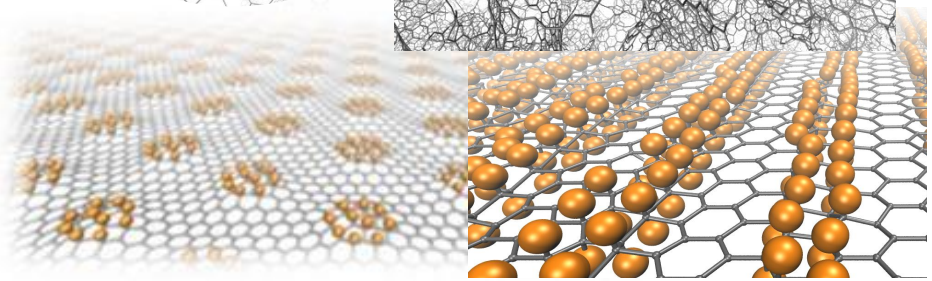
- ✔ The ^{3}H-He potential for the rate calculation depends on loading level and distribution of tritium
- ✔ He detaches and diffuses through the structure
- ✔ Specific vibrational modes are activated that could be detected in coincidence with the decay/capture
- ✔ β electrons may create defects in the material in very specific conditions
- ✔ β electrons interaction and effect depends on tritium loading and distribution and is under study combining MC with MD
- ✔ Simulations are in the course to optimize loading





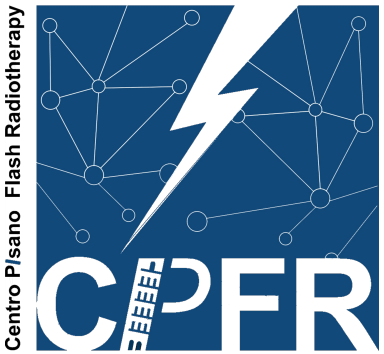


In conclusion, almost each effect depends on the amount and distribution of tritium



Thank you for your attention

Guido Menichetti UniPi, IIT
Angelo Esposito UniRomaI
Andrea Casale Columbia Univ
Luca Bellucci NANO-Cnr
Francesca Maria Pofi GSSI



Electrons interaction with the hydrogenated graphene

(for T at most 15 eV) -> single events cannot generally break a C-C bond but can break a T-C bond

✔ However, the **sub-breaking energy is transferred to the material, which heats up** . With the fluency of EM beams **(fluence ~ 5x10 ^{9} el/nm^{2} sec)** the heat up is fast and defects occurs when local temperature reaches high values.

✔ Secondary electrons effect is not considered in this work, and the Ekin distribution is very roughly described

In our case: we have a probability of decay (and fluence of electrons) that is about **10^{-7} el/nm^{2} sec**) 17 orders of magnitude less -> **fast heat up is certainly not likely**

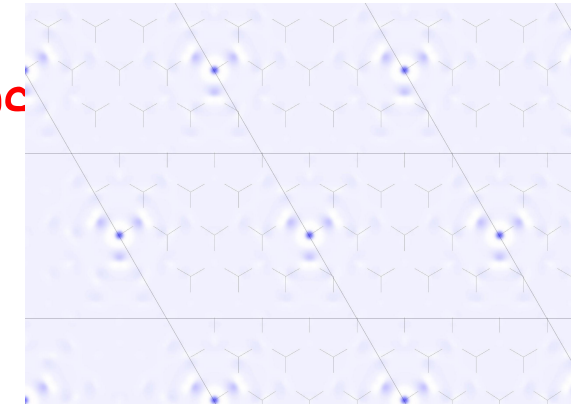
But:

We have additional heating caused by **He release and diffusion within the structure** : each event distributes 2-4 eV of energy per nm^{2} resulting in a heat up of 300-500 K/event = at most 500Kx10^{-7} sec^{-1} (i.e. 300K /year)

C-T bonds can be directly **broken by the primary electrons**

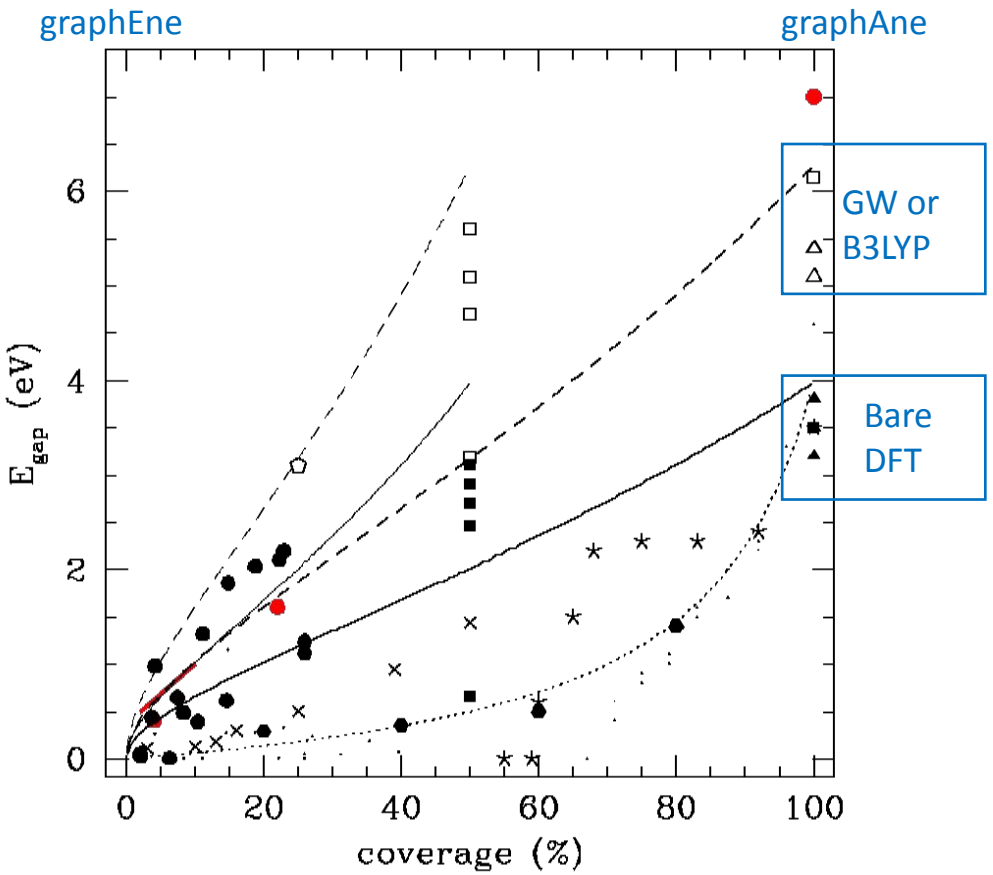
✔ We can properly evaluate the **kinetic energy distribution by MC simulations, inc electrons**

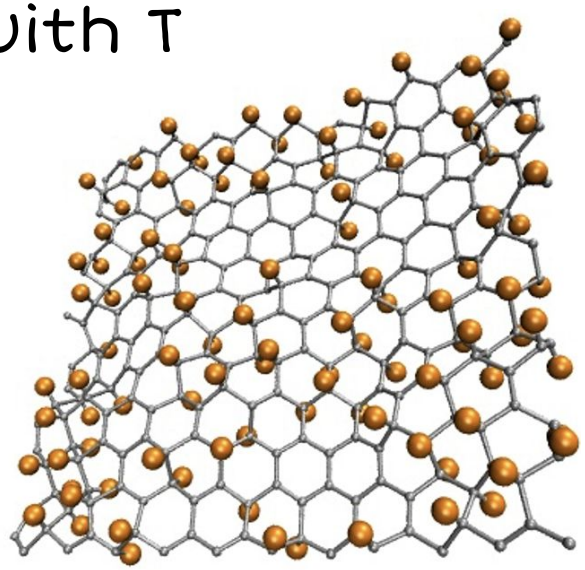
->NEBULA calculations allow to include the material properties.

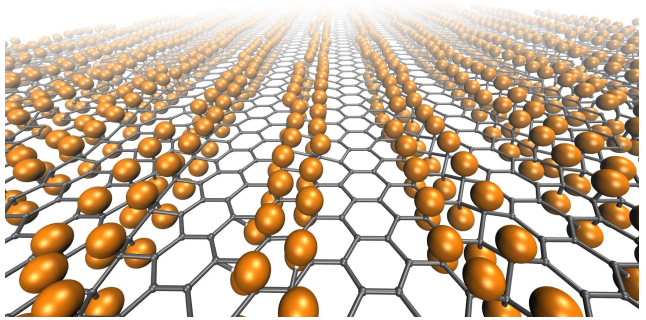


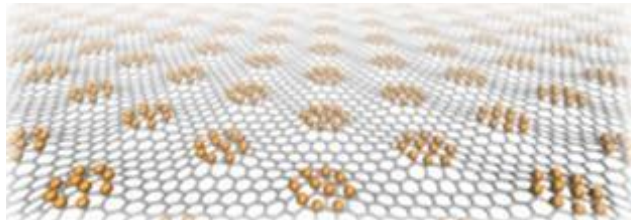
Gap vs coverage

Band gap generally decreases with T loading







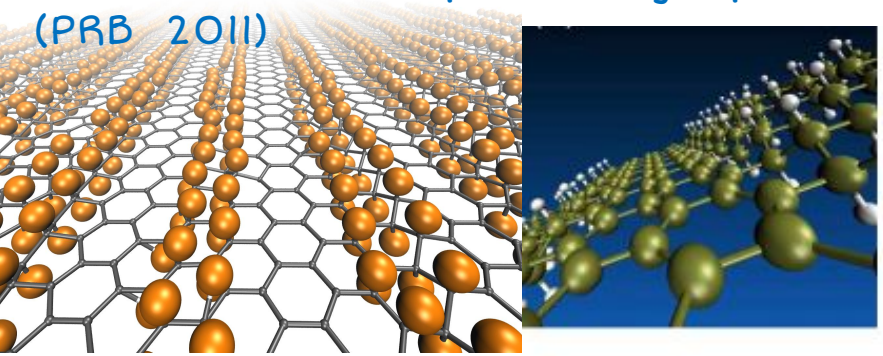


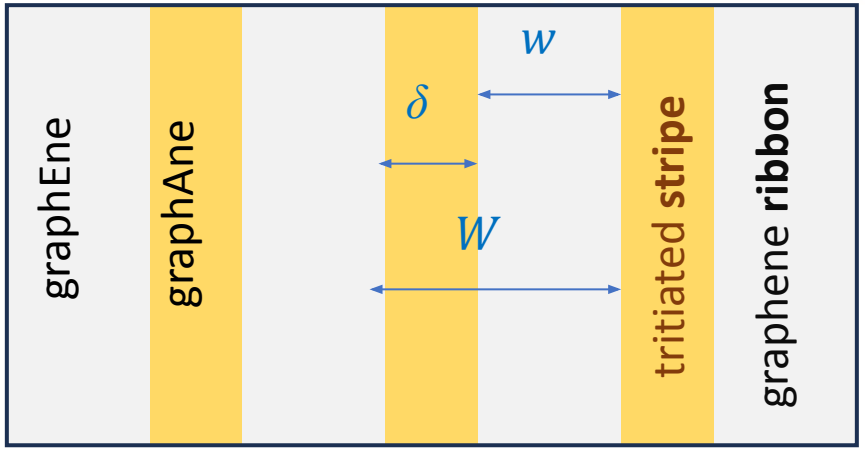
But data from calculations (and exp as well) are very messy mainly because of different hydrogenation modality

- one or two side
- clusters or random
- geometry of hydrogenation (strips, islands, …)

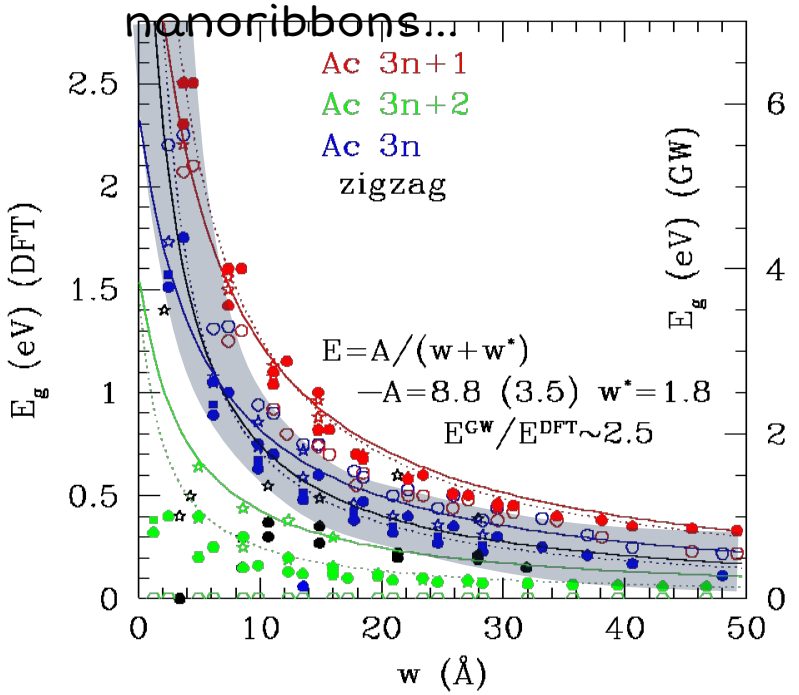
Gap vs coverage: focusing on simple geometries: Tritiation per stripes

Nanoribbons sculpted in graphane (PRB 2011)

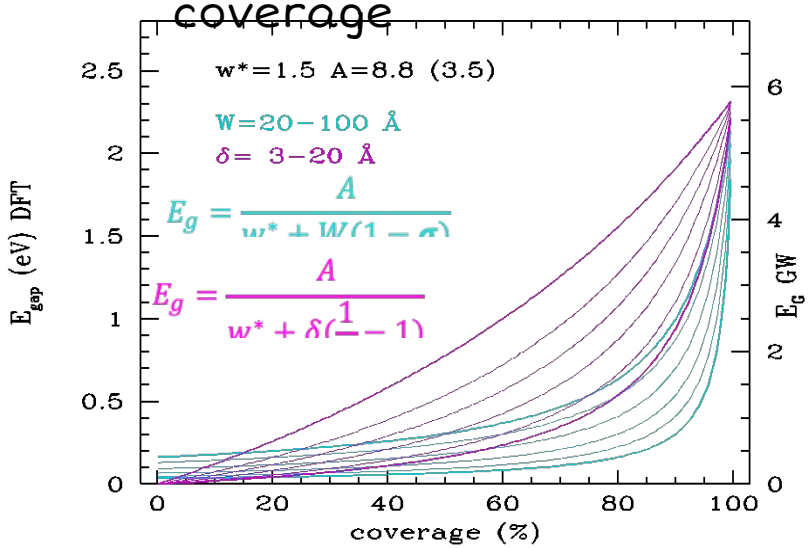


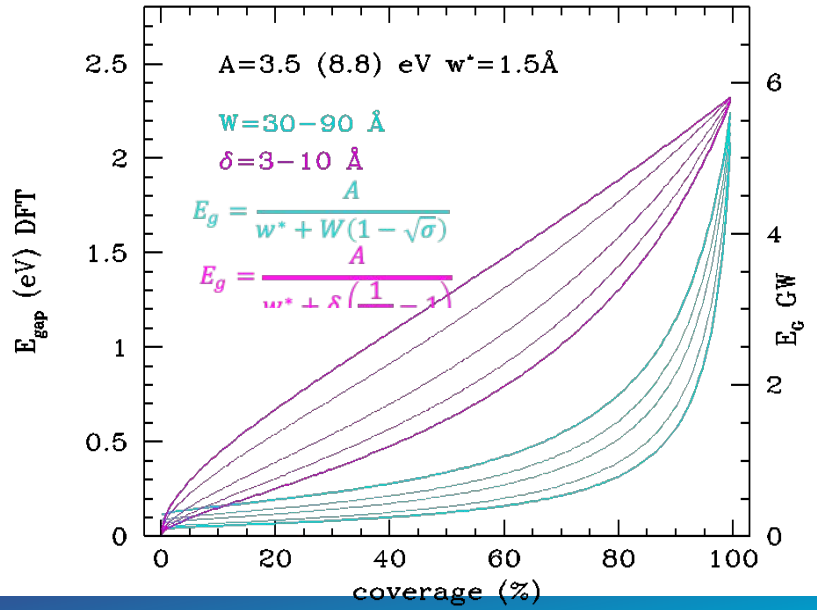


The gap-vs-stripes width dependence is similar to that of graphene nanoribbons...

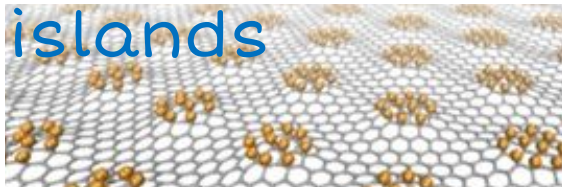


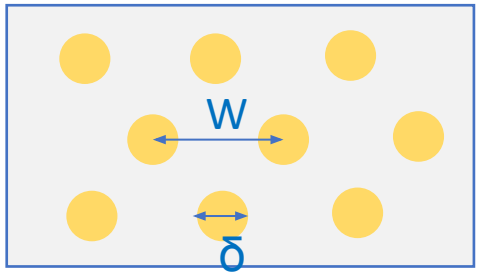
... leading to simple behavior of gap vs coverage





Tritiation per islands

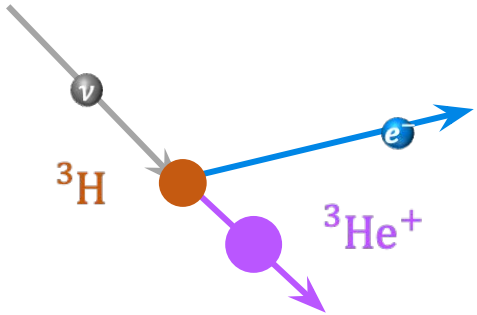




In the per-island tritiation a similar trend can be derived

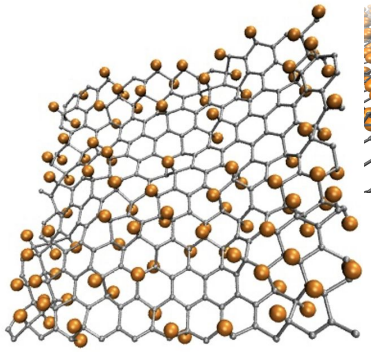
Neutrino capture

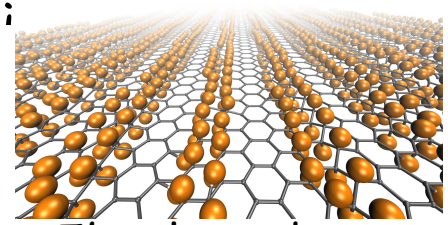
$$\nu_e + {}^3\mathrm{H} \rightarrow {}^3\mathrm{He}^+ + e^-$$

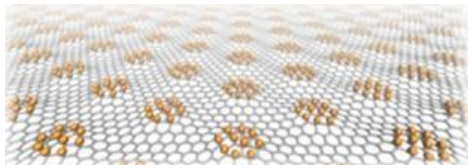


Requirements

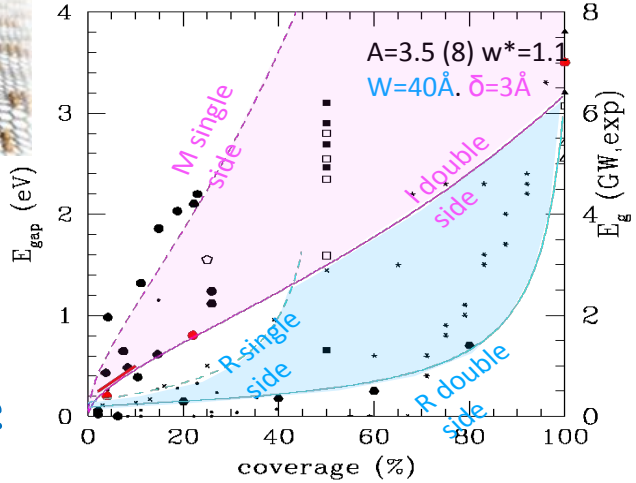
1. The material **must be conductive** for high precision β peak determi

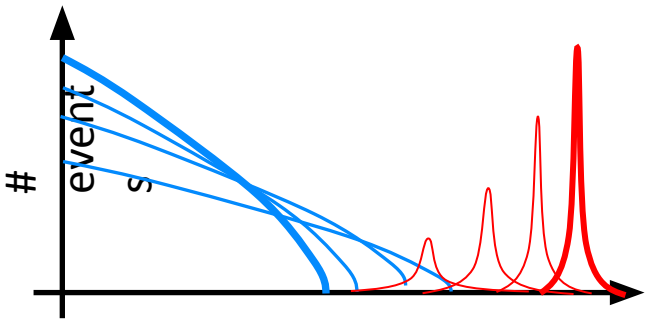






The band gap and conductance depend on distribution of T on graphene

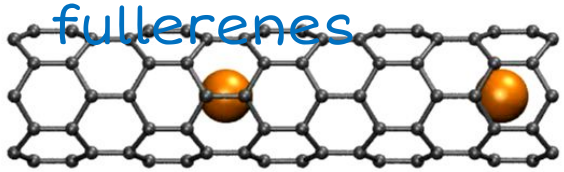


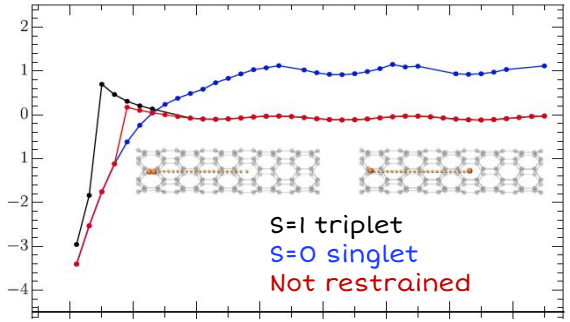


→ **optimization of the material is in the course**

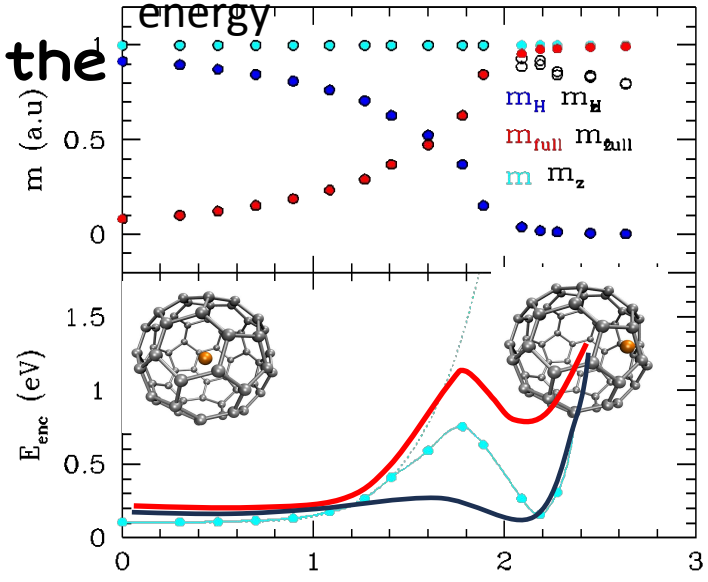
2. The **quantum uncertainty** on the ^{3}H/He momentum **spoils the resolution**

- **The binding potential must be the flattest possible**
  → Encapsulation into nanotubes or fullerenes





- **The ^{3}H/He momentum state must be controlled**
  → excitation of coherent vibrational states



Input for GRAPHITE/graphene: q parallel to plane

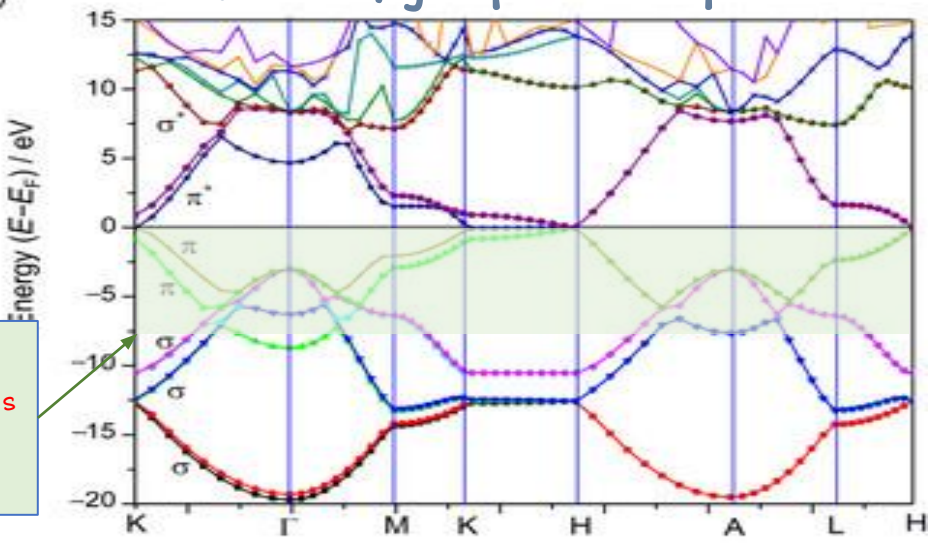
graphite.yaml

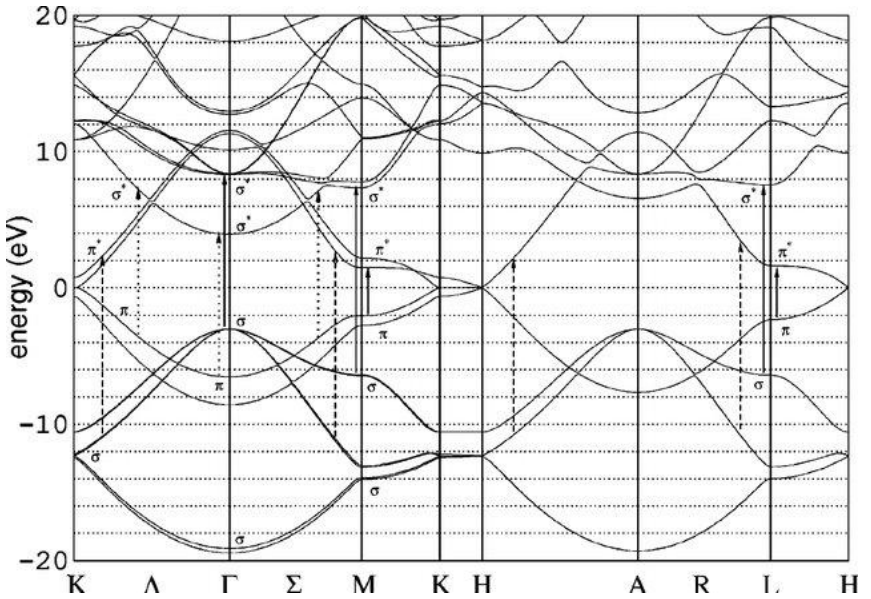
name: graphite
density: 2.2600 g/cm³

elements:
C: { count: 1, Z: 6, M: 12.0116 g/mol }

band_structure:
model: metal
fermi: 7.5 eV
work_function:
4.7-4.8 eV from basal plane, from different literature sources

This is the distance of FL to bottom of conduction band Considering that the pi bands are those contributing more to conduction in plane, I put here the bottom of the main pi bands (average)





optical:
df_file: elf/df_graphite.dat

Discussed in next slides

phonon:
lattice: 2.461 Å
m_dos: 1.0 m_e
m_eff: 0.1 m_e

NB: this is the a lattice constant (**in-plane**) but I'm not really sure what should be put here. First of all, due to anisotropy, the out of plane lattice constant is much larger (6.708). Second, graphite has 2 atoms per cell, and symmetry of the crystal is not given anywhere. Therefore, if one has to put a single value here, that should probably be **1.42, that is the C-C distance**. It is possible that an effective lattice constant to be used for in plane calculation is more around 2 angstrom.

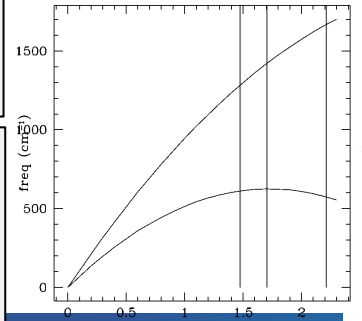
The effective masses m_eff for conduction bands are very small, 0.04-0.05 m_e, but for graphite at K point, the effective mass approximation is poor. In the literature one often finds 0,87, but this is the mass associated to pi-sigma plasmon. Therefore, I'm not even sure of these values. I would try values in the range 0.05-0.5 for the second and ~1 for the first, but we **need to search little more, and see exactly how the parameters are used**

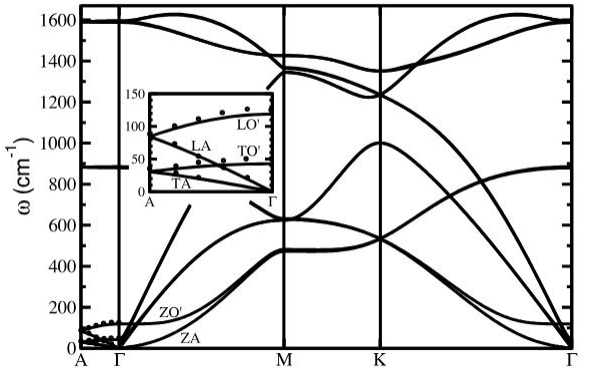
longitudinal:
alpha: 3.0 e-7 m²/s
c_s: 21000 m/s
ac_def: 4.5-6.8-7.8 eV

transversal:
alpha: 4.0 e-7 m²/s
c_s: 13800 m/s
ac_def: 4.5-6.8-7.8 eV

The acoustic **phonon deformation potential ac_def** was taken from estimates on *graphene*, giving effective isotropic values. Therefore the same value is used for the two branches

The **transverse sound speed** is defined only for TA (in plane polarization mode). For the ZA mode (out of plane polarization), it is null, since the dispersion is quadratic. Therefore the effective value of the "transverse sound" velocity may be smaller.
The alpha parmeter (curvature) is set to approximately reproduce the zone boundary acoustic branch bending (see





How does NEBULA represent the material
The case of SILICON

Silicon silicon.yaml

name: silicon
density: 2.3290 g/cm³

elements:
Si: { count: 1, Z: 14, M: 28.0855 g/mol }

band_structure:
model: semiconductor
valence: 7.27 eV
band_gap: 1.12 eV
affinity: 4.05 eV = level of the bottom of conduction bands with respect to vacuum

optical:
df_file: elf/df_Si.dat

phonon:
lattice: 5.430710 Å
m_dos: 1.08 m_e
m_eff: 0.26 m_e

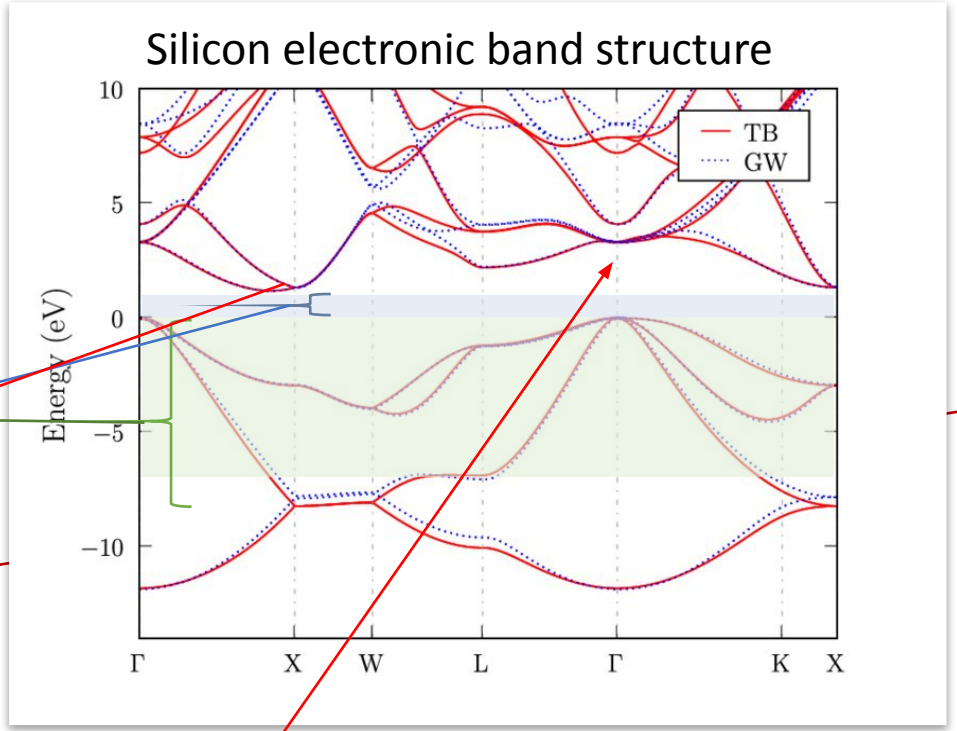
These effective masses are the curvature of bands (average) of valence and conduction bands for electron damping by phonons calculations

longitudinal:
alpha: 2.00e-7 m²/s
c_s: 9130 m/s # Landolt-Bornstein Vol. III/41A1a 872
ac_def: 9.2 eV # Landolt-Bornstein Vol. III/41A1a 648

Curvature parameter at zone boundary

Linear part coefficients

transversal:
alpha: 2.26e-7 m²/s
c_s: 5842 m/s # Landolt-Bornstein Vol. III/41A1a 872
ac_def: 5.0 eV # Landolt-Bornstein Vol. III/41A1a 648



How optical properties are treated

1. The q dependent ELF is expanded from that at q=0 in terms of the Lindhard function

$$\mathrm{Im}\left[\frac{-1}{\varepsilon(q,\omega)}\right]=\int_0^\infty d\omega_p g(\omega_p)\mathrm{Im}\left[\frac{-1}{\varepsilon_L(q,\omega;\omega_p)}\right]$$

$$\varepsilon_L(q,\omega;\omega_p)$$

$$g(\omega)=\frac{2}{\pi\omega}\mathrm{Im}\left[\frac{-1}{\varepsilon(\omega)}\right]$$

$$\varepsilon_L^r=1+\frac{1}{\pi k_F}\frac{1}{Z^2}\left[\frac{1}{2}+\frac{1}{8Z}F\left(Z-\frac{X}{4Z}\right)+\frac{1}{8Z}F\left(Z+\frac{X}{4Z}\right)\right],$$

$$\varepsilon_L^i=\begin{cases}\frac{1}{8k_F}\frac{X}{Z^3}, & 0\leqslant X\leqslant 4Z(1-Z);\\ \frac{1}{8k_F}\frac{1}{Z^3}\left[1-\left(Z-\frac{X}{4Z}\right)^2\right], & |4Z(1-Z)|\leqslant X\leqslant 4Z(1+Z)\\ 0, & \text{otherwise,}\end{cases}$$

2. The lindhard function is approximated by sin

$$\mathrm{Im}\left[\frac{-1}{\varepsilon_L(q,\omega;\omega_p)}\right]\approx\frac{\pi}{2}\frac{\omega_p^2}{\omega_q}\delta(\omega-\omega_q)$$

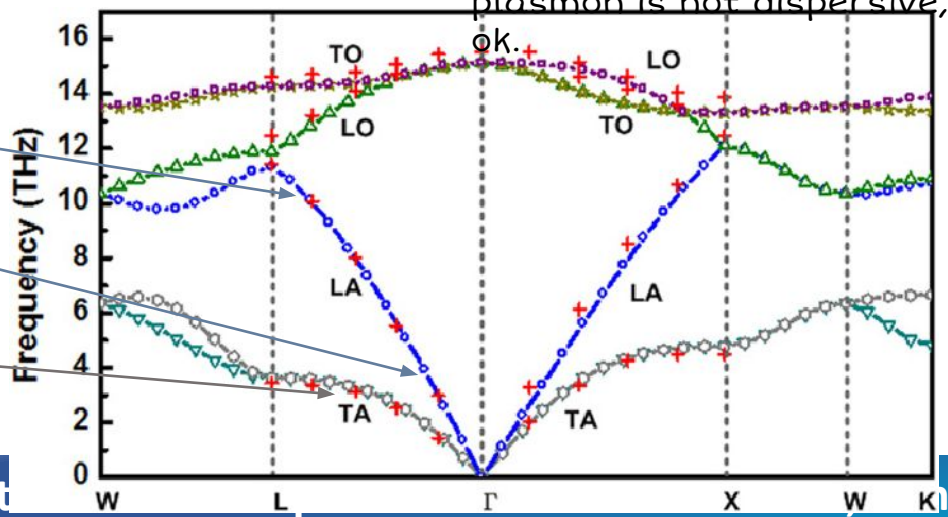
leading to

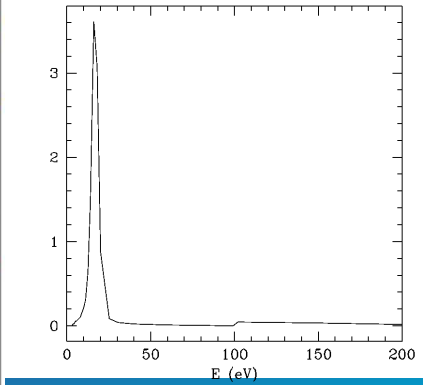
$$\mathrm{Im}\left[\frac{-1}{\varepsilon(q,\omega)}\right]\approx\frac{\omega_0}{\omega_q}\mathrm{Im}\left[\frac{-1}{\varepsilon(\omega_0)}\right]$$

with

ω_0 is the solution of the equation $\omega_q(\omega_0)=\omega$.

All depends on the optical epsilon and on the dispersion of plasmons (one or more), and serves to approximate the real epsilon(q,omega) when it is not known. If the plasmon is not dispersive, the q=0 approx is ok.





Density Functional Theory calculations

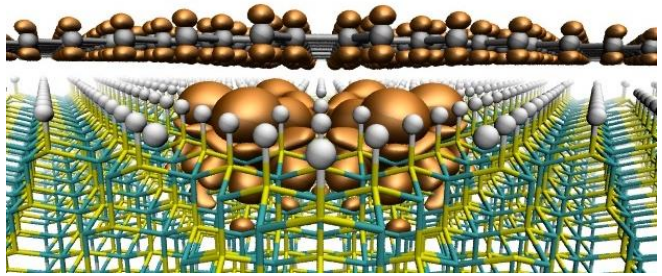
✔ Density Functional Theory

$$E[n,\mathbf{R}] = E_k[n] + E_{xc}[n] + E_H[n] + \int V_N(\mathbf{R},\mathbf{r})n(\mathbf{r})d\mathbf{r} + E_{NN}(\mathbf{R})$$

- ➔ BO → self consistent calculation for *n* at given **R**
- ➔ Frozen electrons: non self consistent calculation at given n with variable **R**

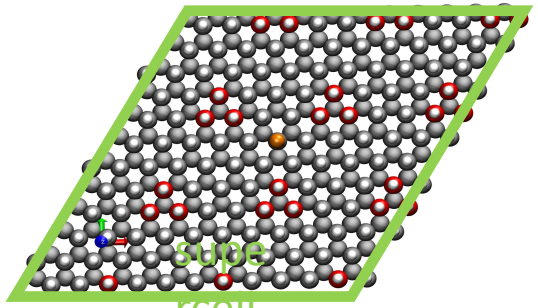
✔ Calculations

- ➔ **Electron density** $\rho(r)$ and **full electronic structure** → Bands&gaps, Fermi level, optical properties, transport…
- ➔ **Electron spin density** $\zeta(r)$ → magnetism
- ➔ **Forces on nuclei** → vibrational properties and molecular dynamics

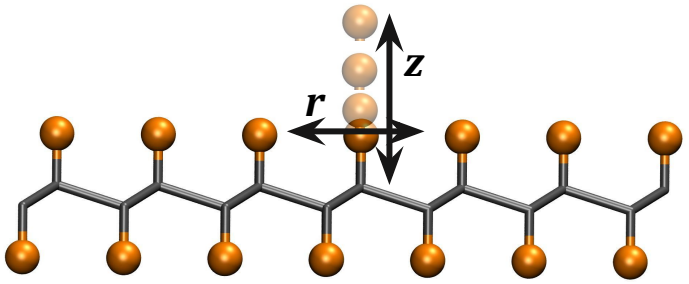


✔ Calculation setup

- ➔ Density Functional $E_{xc}[n(r)]$ = **Generalized Gradient Corrected** (PBE) + vdW correction + spin resolved
- ➔ Augmented Plane Wave expansion (periodic boundary conditions) Quantum Espresso Code, vs 7.2
- ➔ Steered, damped or free molecular dynamics for the conformational space exploration
- ➔ Run on Leonardo@CINECA 4-8 nodes (4 GPUxnode, 32 core x node) → 128-256 Cores, 14-24 GPUs, or local nodes (test calculations)



Focus on the beta decay

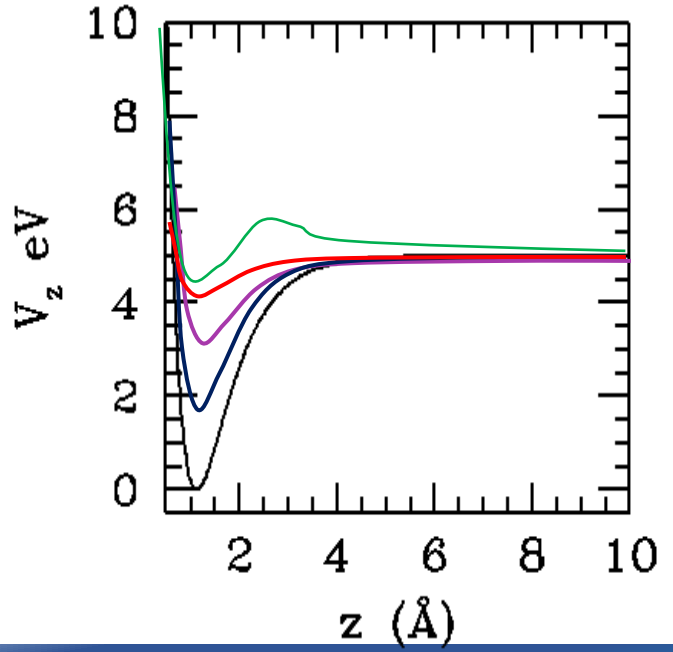


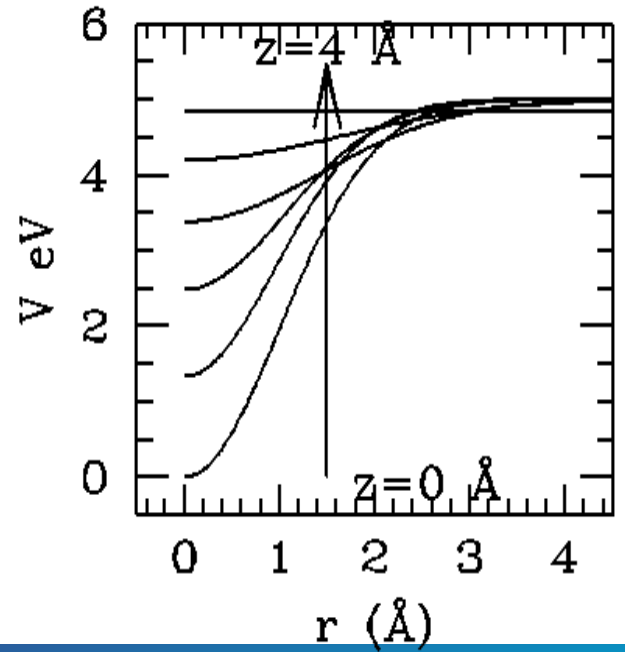
$$^3\mathrm{H} \rightarrow {}^3\mathrm{He}^+ + e^- + \bar{\nu}_e$$

$$M \sim \int d\mathbf{x}\, \Psi_0\, \Psi_f^* e^{i\mathbf{p_{el}}\cdot\mathbf{x}}$$

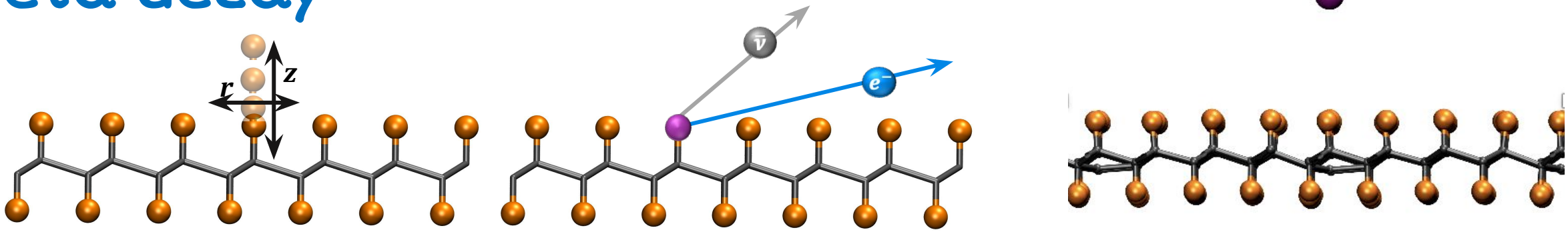
Starting state Ψ_0 : T is relaxed on the substrate

- ✓ **BO** standard DFT for evaluation of **orthogonal and lateral potential**
- ✔ The **binding energy** depends **on loading level and distribution,** and on the local geometry of the substrate
- ✔ A **barrier** can be present especially in presence of spin polarization or in concavities

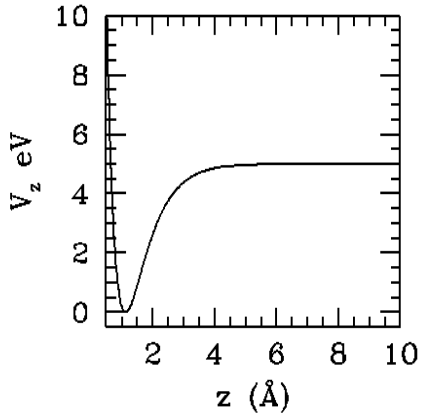


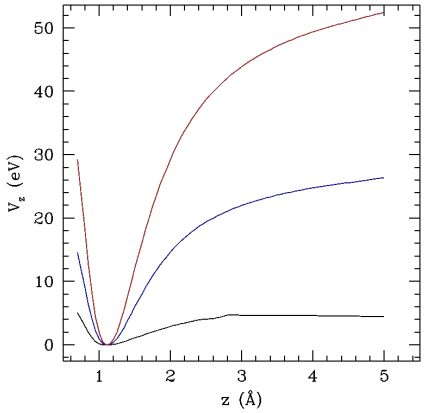


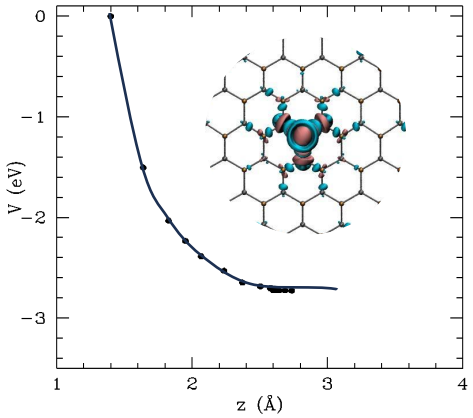
Beta decay

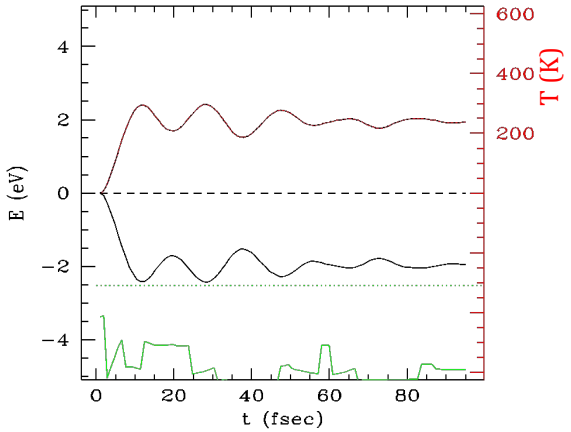


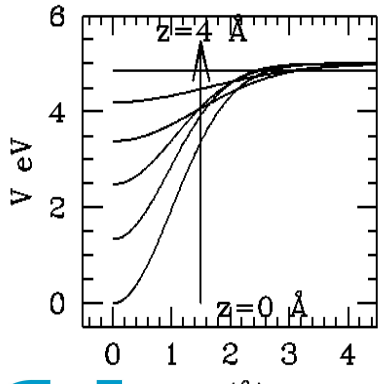
t=0 t~fs t~ps-ns



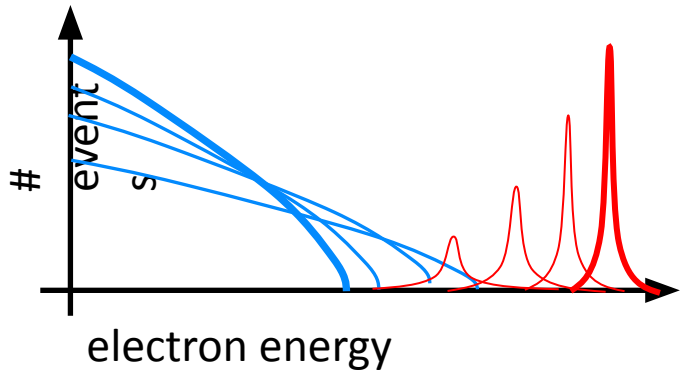








The accurate evaluation of potentials at different stages allow evaluating the β emission spectra endpoint with high precision

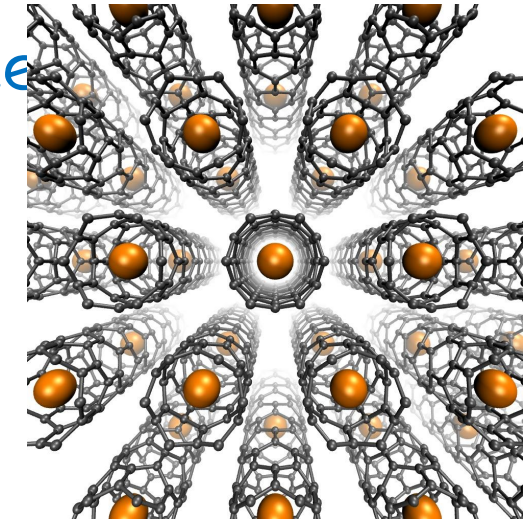


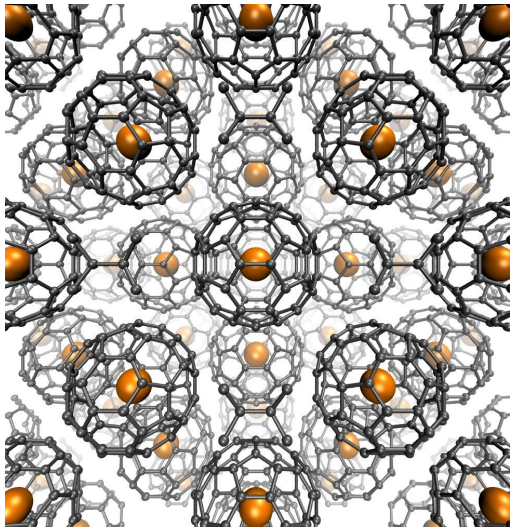
→ neutrino

Neutrino capture and quantum tech

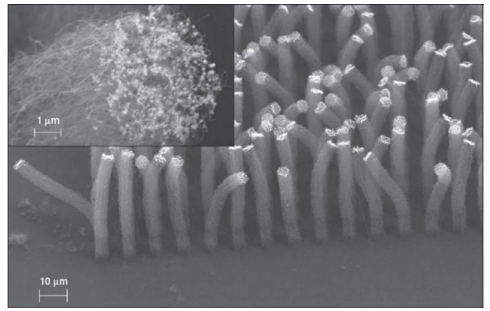
➔ Encapsulation into nanotubes or fulle

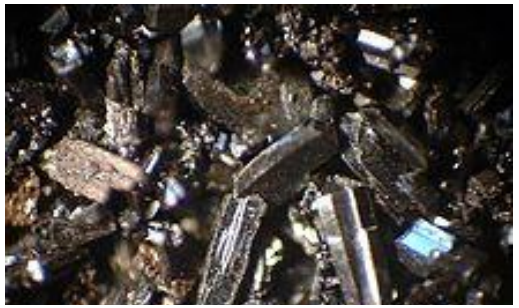
The need for high concentration of tritium can be recovered compacting tubes into **bundles** or fullerene into **fullerite**

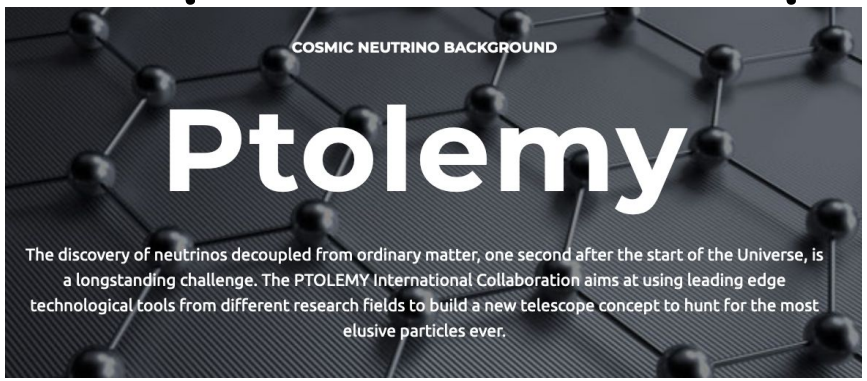




➔ These systems are also considered as bases for **quantum bits encoded into the encapsulated atom spin**





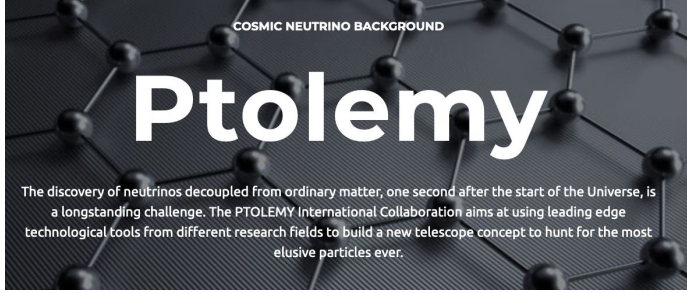


PHYSICAL REVIEW D **106,** 053002 (2022)

Heisenberg's uncertainty principle in the PTOLEMY project: A theory update

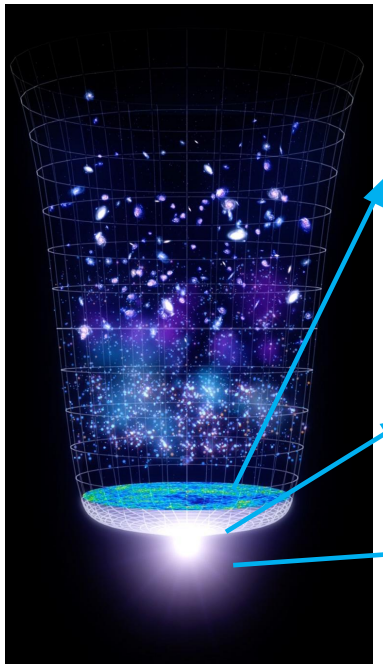
A. Apponi,[1,2] M. G. Betti,[3,4] M. Borghesi,[5,6] A. Boyarsky,[7] N. Canci,[8] G. Cavoto,[3,4] C. Chang,[9,10] V. Cheianov,[7] Y. Cheipesh,[7] W. Chung,[11] A. G. Cocco,[12] A. P. Colijn,[13,14] N. D'Ambrosio,[8] N. de Groot,[15] A. Esposito,[16] M. Faverzani,[5,6] A. Ferella,[8,17] E. Ferri,[5] L. Ficcadenti,[3,4] T. Frederico,[18] S. Gariazzo,[19] F. Gatti,[20] C. Gentile,[21] A. Giachero,[5,6] Y. Hochberg,[22] Y. Kahn,[10,23] M. Lisanti,[11] G. Mangano,[12,24] L. E. Marcucci,[25,26] C. Mariani,[3,4] M. Marques,[18] G. Menichetti,[26,27] M. Messina,[8] O. Mikulenko,[7] E. Monticone,[19,28] A. Nucciotti,[5,6] D. Orlandi,[8] F. Pandolfi,[3] S. Parlati,[8] C. Pepe,[19,28,29] C. Pérez de los Heros,[30] O. Pisanti,[12,24] M. Polini,[26,31,32] A. D. Polosa,[3,4] A. Puiu,[8,33] I. Rago,[3,4] Y. Raitses,[21] M. Rajteri,[19,28] N. Rossi,[8] K. Rozwadowska,[8,33] I. Rucandio,[34] A. Ruocco,[1,2] C. F. Strid,[35] A. Tan,[11] L. K. Teles,[18] V. Tozzini,[36] C. G. Tully,[11] M. Viviani,[25] U. Zeitler,[15] and F. Zhao[11]

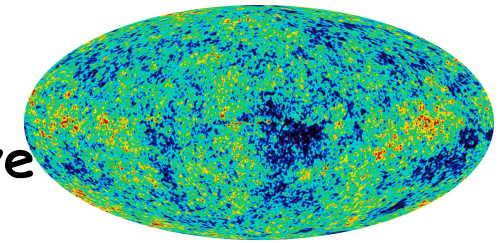
Neutrin ... are "elusive" and "informative"



os

- Their mass is "almost" null and unknown (0.5-0.8 eV)
- ✔ They are neutral and interact only "wealkly" with other particles
- ✔ Their cosmic background bears extremely interesting information on the early universe (decoupled 1 sec after Big Bang)





Microwave cosmic background (> 380Kyears, 2.7K)

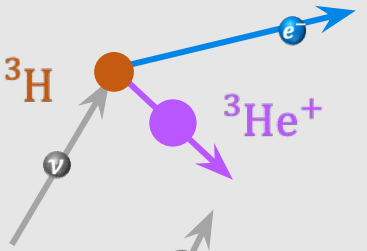
Gravitational wave cosmic background (VIRGO)

1 sec after Big Bang
Relic neutrinos background
(density ~53 cm^{-3}, energy~10^{-4} eV)

- ✔ Interaction with Tritium (^3H) to explore neutrinos

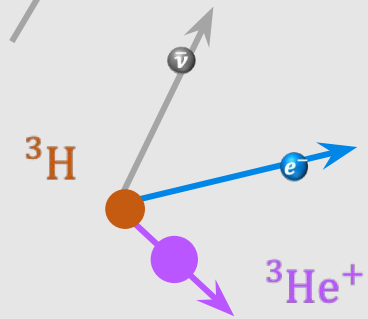
- Neutrino capture

$$\nu_e + {}^3\mathrm{H} \rightarrow {}^3\mathrm{He}^+ + e^-$$



- Tritium β decay

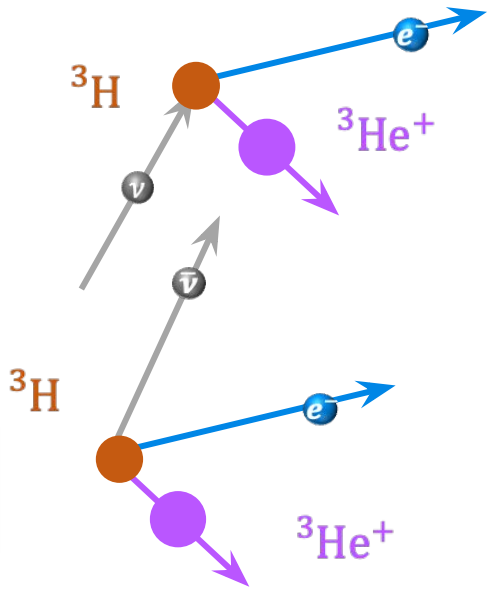
$$^3\mathrm{H} \rightarrow {}^3\mathrm{He}^+ + e^- + \bar{\nu}_e$$



Neutrinos interaction with Tritium

- Neutrino capture

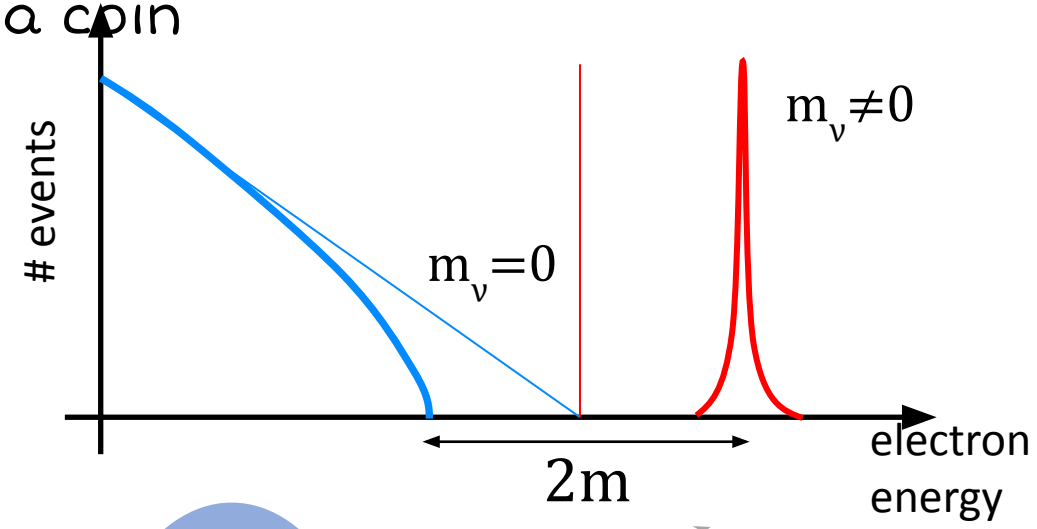
$$\nu_e + {}^3\mathrm{H} \rightarrow {}^3\mathrm{He}^+ + e^-$$

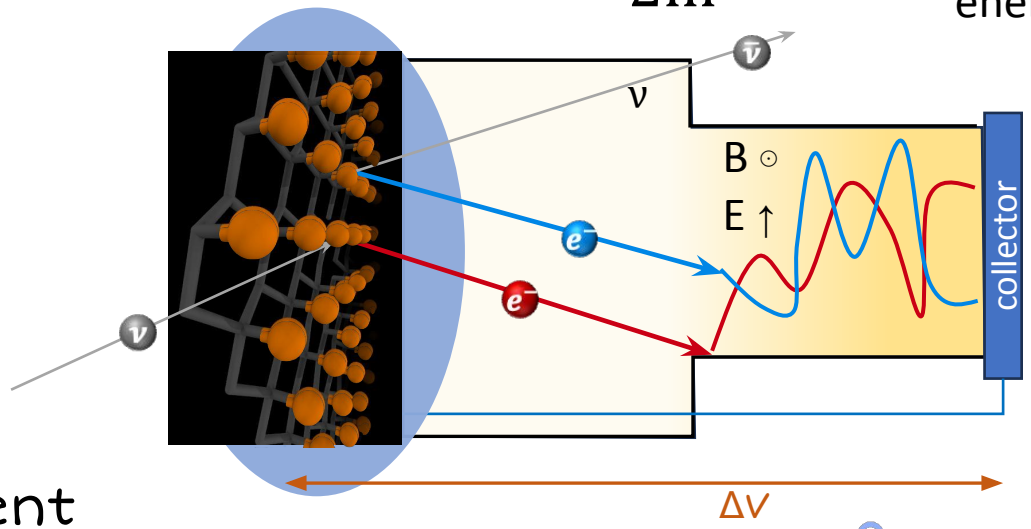


- Tritium β decay

$$^3\mathrm{H} \rightarrow {}^3\mathrm{He}^+ + e^- + \bar{\nu}_e$$

Capture and decay: two faces of a coin





✔ Both process can measure **neutrino mass**

✔ Capture can detect the **relic neutrinos**

The detector needs

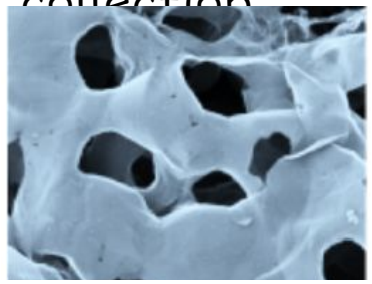
- **High concentration** of tritium for high event rate
- **High exposure** of tritium for efficient e^- collection
- **Conducting material** for accuracy in energy measurement

Tritium on graphene!

PTOLEMY

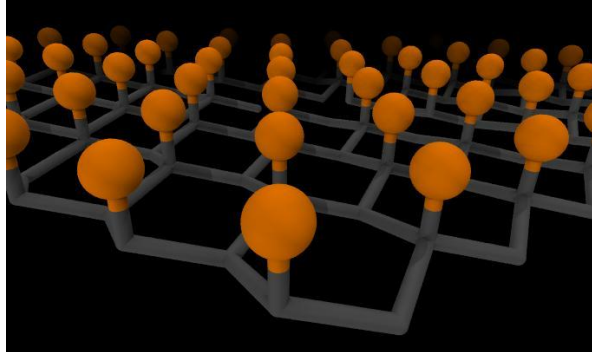
Tritium on graphene

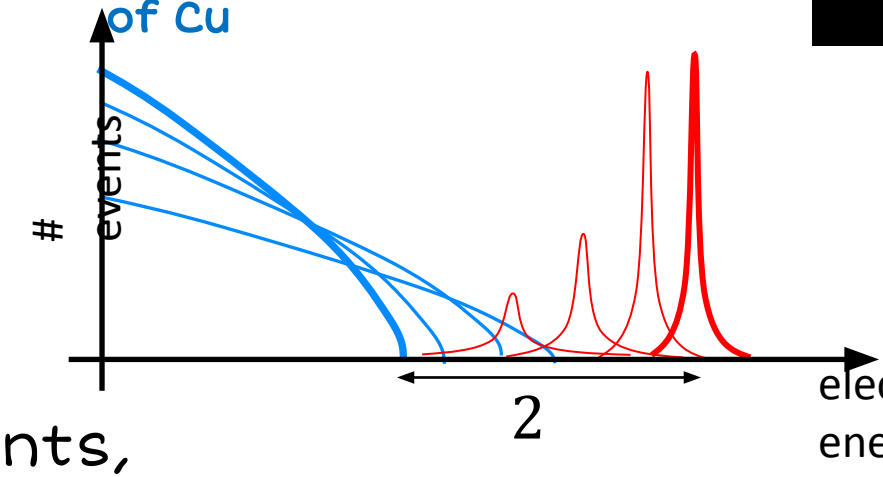
- **High concentration** of tritium for high event rate
- **High exposure** of tritium for efficient e^- collection
- **…terial** for accuracy in energy



Nanoporous graphene can be loaded up to 90%
Betti et al Nanolett 2024

0.019 μg/cm² = **0.19mg/m²**
0.1g/cm³ = **100 kg/m³**
Accessible surface **2630 m²/g**
High electron mobility **x 1000 of Cu**





- Neutrino captu

$$\nu_e + {}^3\mathrm{H} \rightarrow {}^3\mathrm{He}^+ + e^-$$

- Tritium β decay

$$^3\mathrm{H} \rightarrow {}^3\mathrm{He}^+ + e^- + \bar{\nu}_e$$

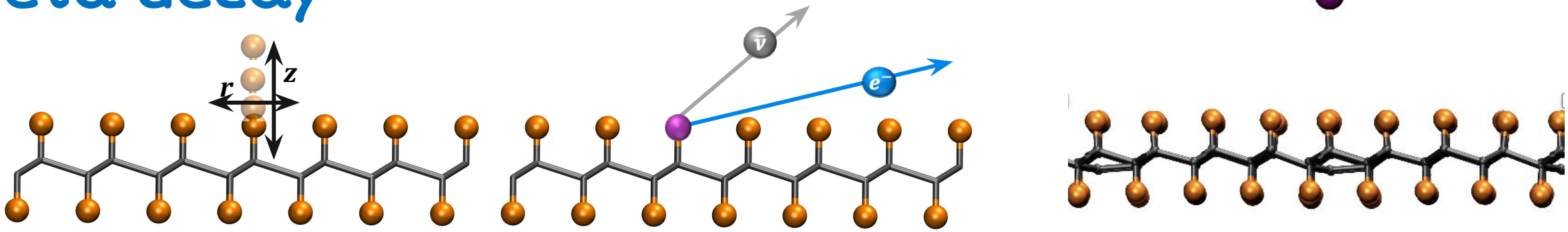
Graphene satisfies the requirements,
BUT…
The substrate effects must be included in the reactions!

$$M \sim \int d\mathbf{x}\, \Psi_0\, \Psi_f^* e^{i\mathbf{p_{el}}\cdot\mathbf{x}}$$

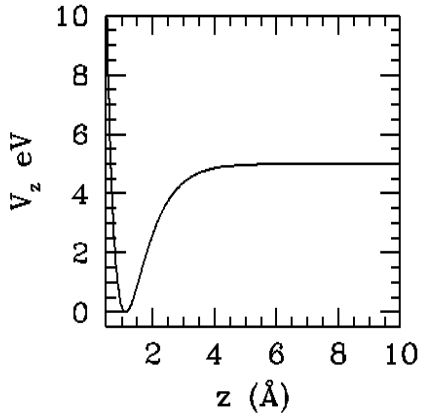
- ✓ $\Psi_0(^3H)$ **and** $\Psi_f(^3He^+)$ are influenced by the substrate
- ✓ The **spectra turns out considerably different** from the case *in vacuo*
- ✓ The **interaction potential** of H/He^+ with graphene must be known **with high precision**
- ✓ The **conduction properties** of the material must be known during reactions

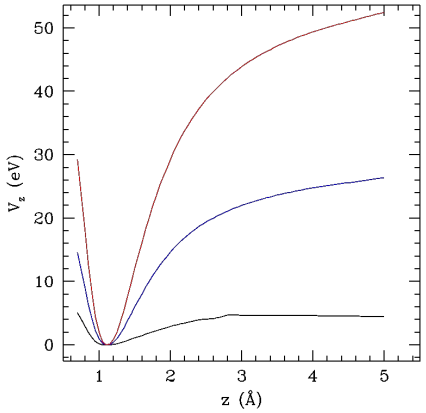
→ **Density Functional Theory calculations in non-standard conditions**

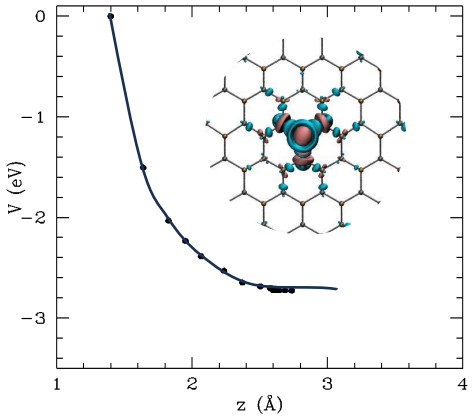
Beta decay

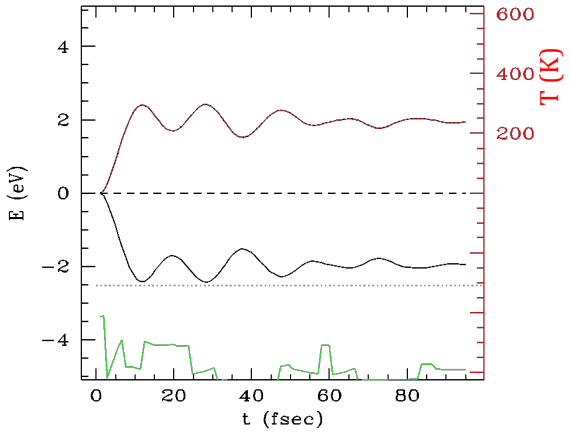


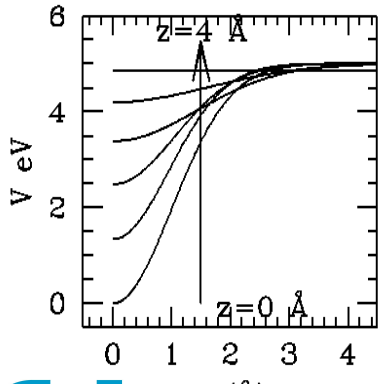
t=0 t~fs t~ps-ns



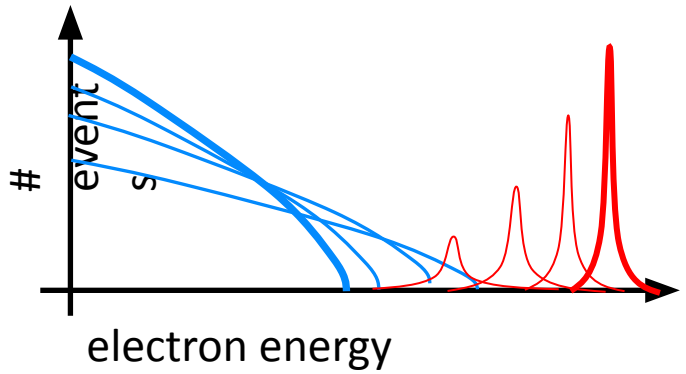








The accurate evaluation of potentials at different stages allow evaluating the β emission spectra endpoint with high precision



→ neutrino