Tritium encapsulation within fullerite, calculations

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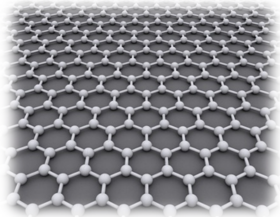
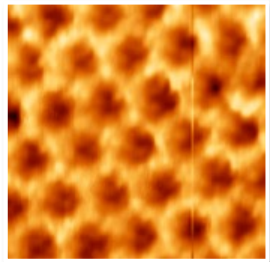
Outline

- ✓ Interaction of T with graphenes
- ✓ Our focus: hollow encapsulated fullerenes
- ✓ Nanotubes
- ✓ Fullerenes

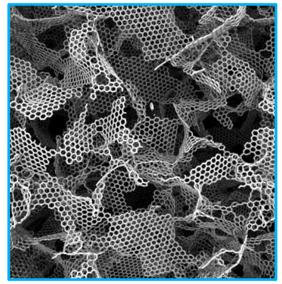
Why graphene-based systems as tritium support?

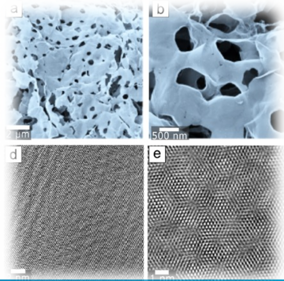
✓ Graphene related materials are very light, resistant and porous and can in principle store a large amount of tritium





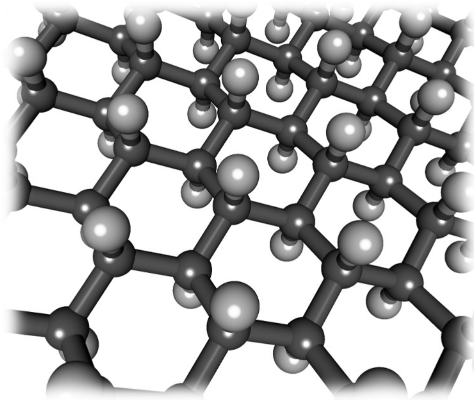
system	Binding strength	Env conditions	density
Vacuum, T_2	Very strong ($\kappa \sim 9$ eV/Å^2)	Any	Up to 0.21 g/cm^3
Vacuum, T_2^*	Less strong ($\kappa \sim 2$ eV/Å^2)	Electronic excited state	
Vacuum, T	null	T ~0.3 K, B ~10 T	~0.5 g/m^3=. 0.5μg/cm^3
T:graphene	Less strong ($\kappa \sim$ 1.5-4 eV/Å^2)	Any	Up to 1.7 μg/cm^2 ~**0.17g/cm^3 (graphAne)**
T@fullerite	Weak	Any; No B	Up to ~0.0036 g/cm^3 = **3.6 mg/cm^3**
T@nanotube	Weak along the axis	Any weak B	Up to ~0.02g/cm^3 = 20 mg/cm^3



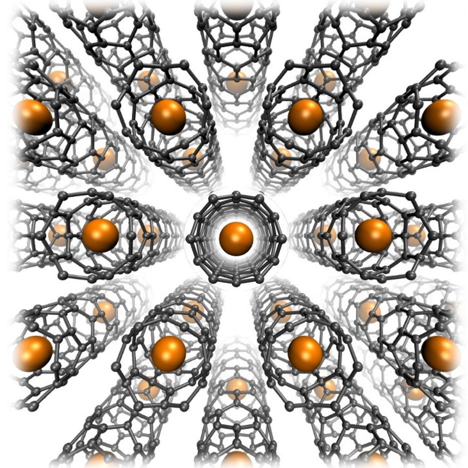


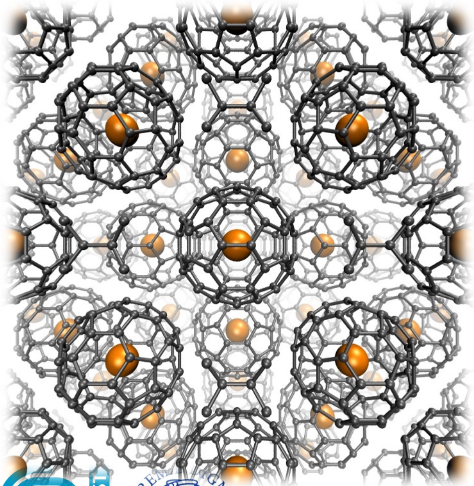
✓ By chemical binding Tritium can be stored in ATOMIC form

✓ But: chemical bonding creates problems for the detection resolution

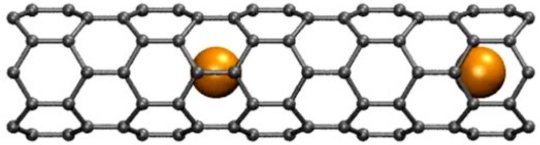


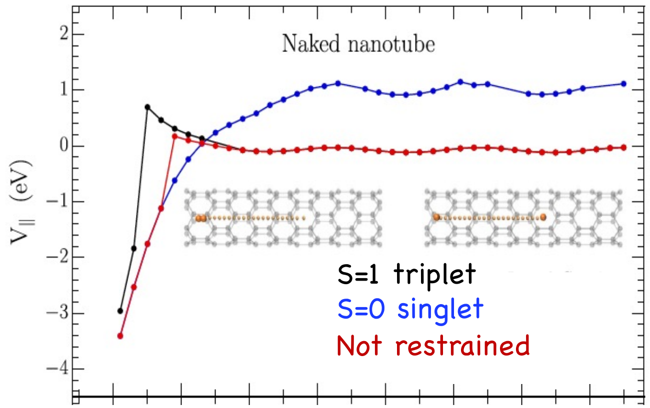
Encapsulated hollow graphenes: nanotubes and fullerenes

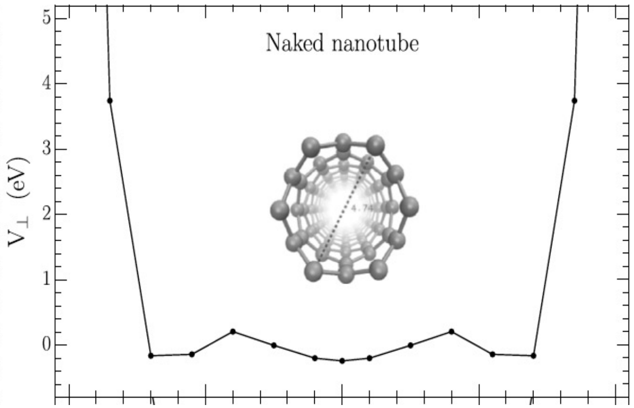


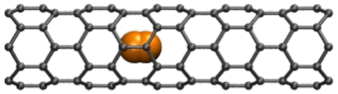


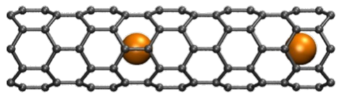
- ✓ Can encapsulate T
- ✓ Can be compacted in bundles (tubes) or in crystal (fullerite) to achieve quite high T density
- ✓ Nanotubes: T dimerization can be avoided, with the aid of small magnetic fields



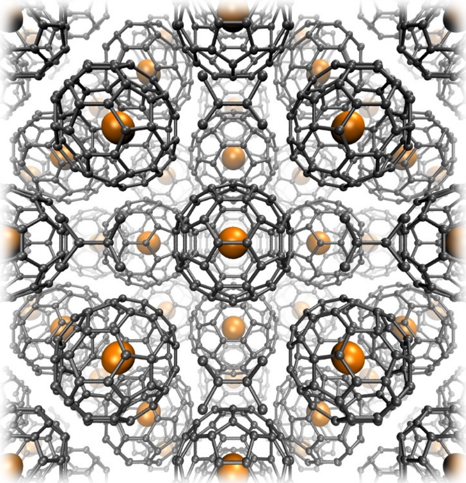


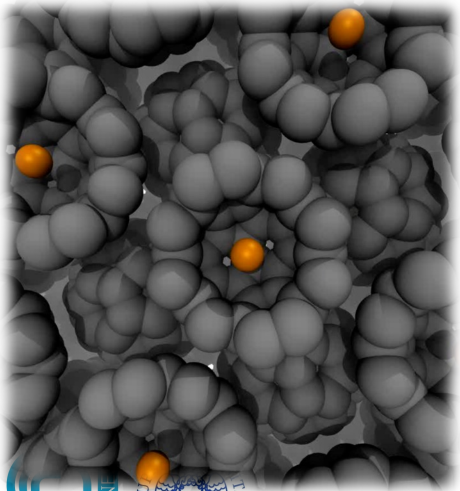


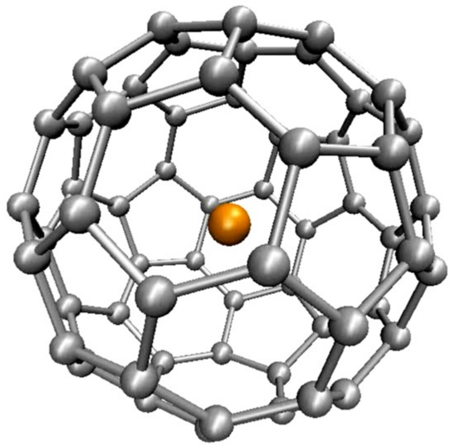




Encapsulated fullerenes in fullerite

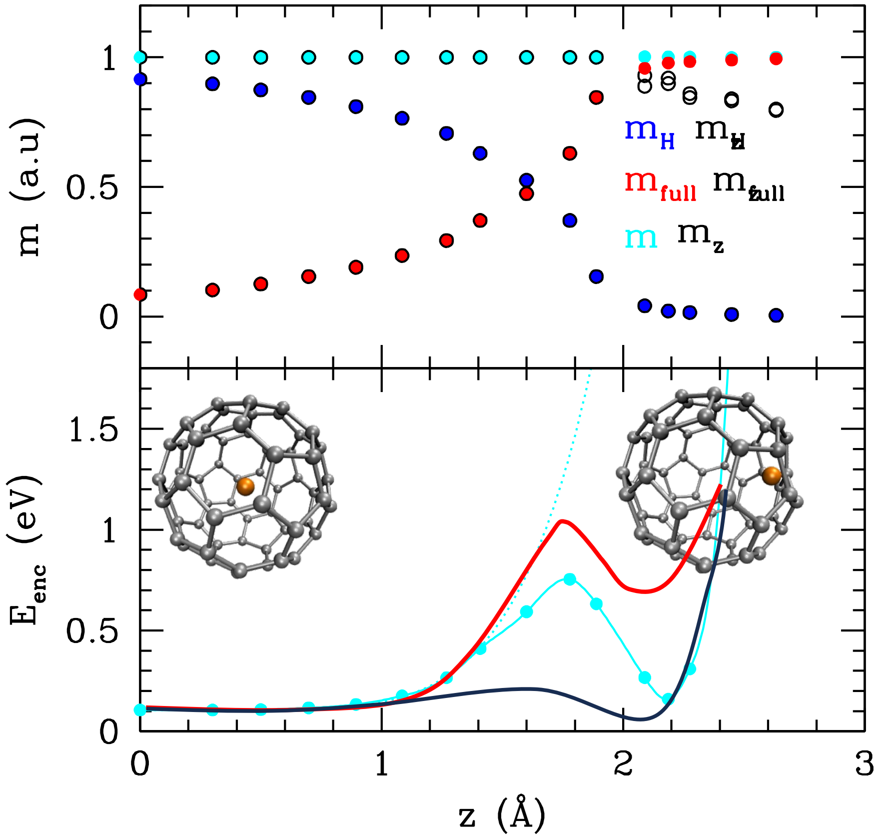






- ✓ Within crystal, the spin of encapsulated T can alter the relative stability of the bound/unbound state

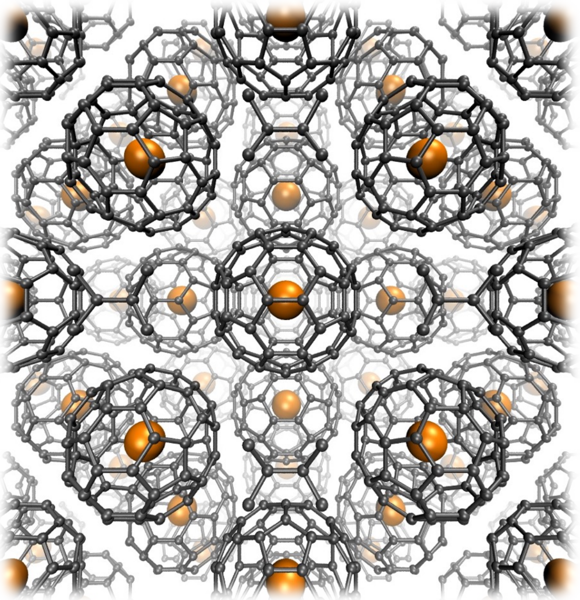
- ✓ Isolated fullerene: During binding, the spin state of the system changes



Encapsulated fullerenes in fullerite

Project Title

Title	*Structural, Electronic and magnetic properties of Tritium Encapsulated fullerite for high energy and quantum computing applications*
Acronym	*SETE*
Project category	*Scalable computing: Scientific use cases that require higly parallel jobs on large scale HPC architectures*



The evaluation requires HPC resources for a full multi-scale approach. Obtained an **ISCRA-C @CINECA for 240K GPUcore hours (Tozzini-Menichetti)** to

- ✓ Evaluate the relative stability of bound-unbound states within the crystal, for **different occupation**
- ✓ Evaluate the **effect if spin interactions** on the profile
- ✓ Study the **vibrational properties** of the system at different temperatures
- ✓ Evaluate **excited states profiles and energy loss spectra**
- ✓ Study the possibility of explointing the resonance with **coherent vibrational states**
- ✓ …

Summary

- ✓ Small nanotubes can store large amount of T, which could be kept in atomic form, almost free along the tube axis (with the aid of a weak magnetic field)
- ✓ T in fullerite can spontaneously live in atomic form in fullerite
- ✓ Its stability can be modulated by the intrinsic spin interaction
- ✓ The interplay with the vibrational resonances is also under study
- ✓ Within the same protocol also other system could be studied, such as nanoporous graphenes with encapsulated T or T@C60
- ✓ The study is currently in the course under a just granted HPC project SETE