STATUS OF THE INTRINSIC QUANTUM SPREAD ON DIFFERENT CARBON SUBSTRATES

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OUTLINE

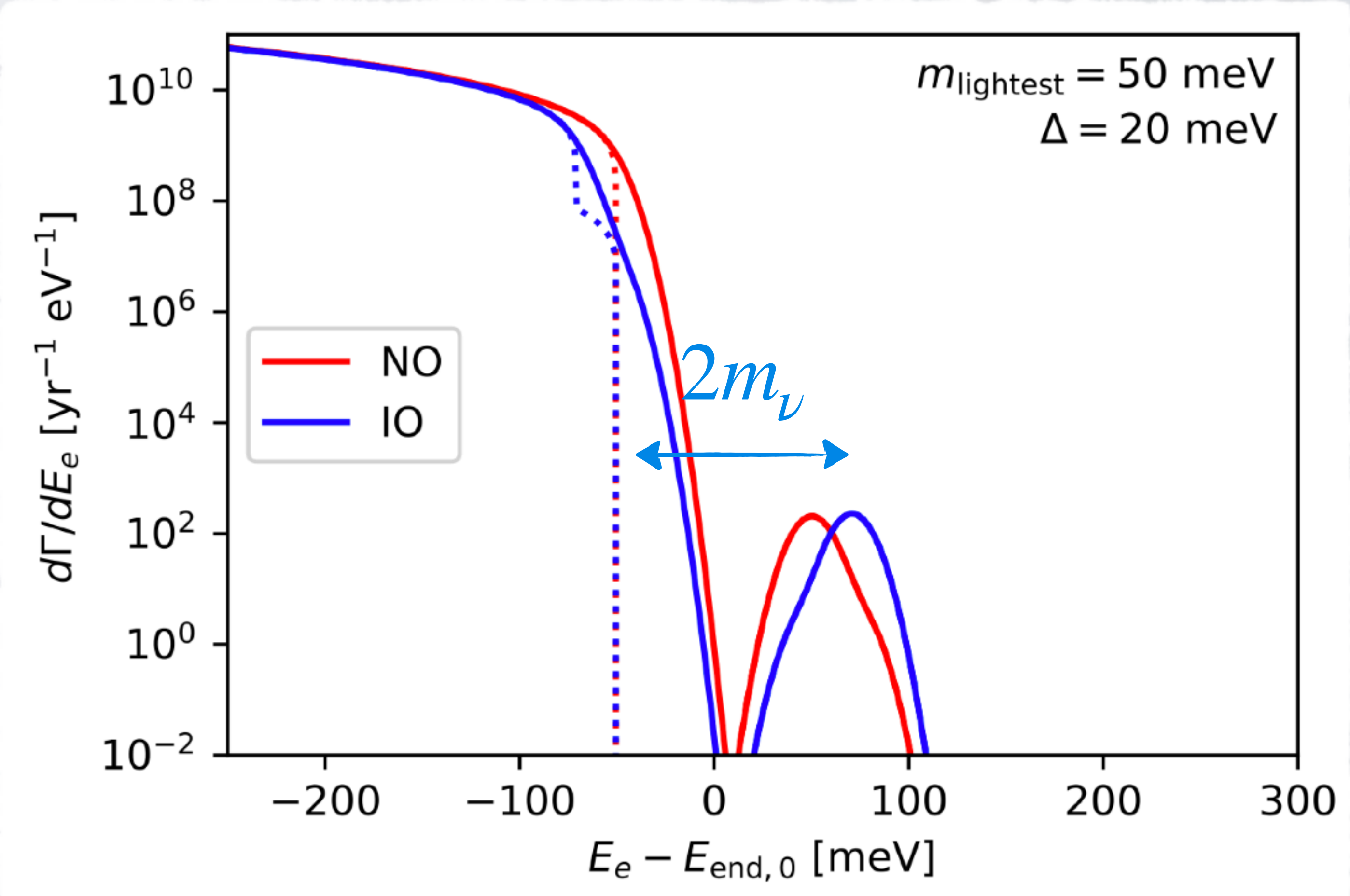
- Super quick recap of the quantum spread issue
- Carbon nanotubes
- Preliminary results on C_{60} fullerenes
- Outlook

RECAP OF THE ISSUE

- One of the goals of Ptolemy is to hunt for the cosmic neutrino via the absorption process: $\nu_e + {}^3\mathrm{H} \to {}^3\mathrm{He}^+ + e^-$

- Expectation in vacuum:

- Cosmic neutrino absorption appears as a peak distant from the β-decay end-point roughly $2m_\nu$



RECAP OF THE ISSUE

- On a substrate the tritium is spatially localized $\longrightarrow$ zero-point motion induces an intrinsic spread in the electron energy

$$\Delta K_e \simeq \left| \frac{\mathbf{p}_e \cdot \Delta \mathbf{p}_T}{m_{He}} \right| \sim 0.82 \text{ eV for graphane}$$

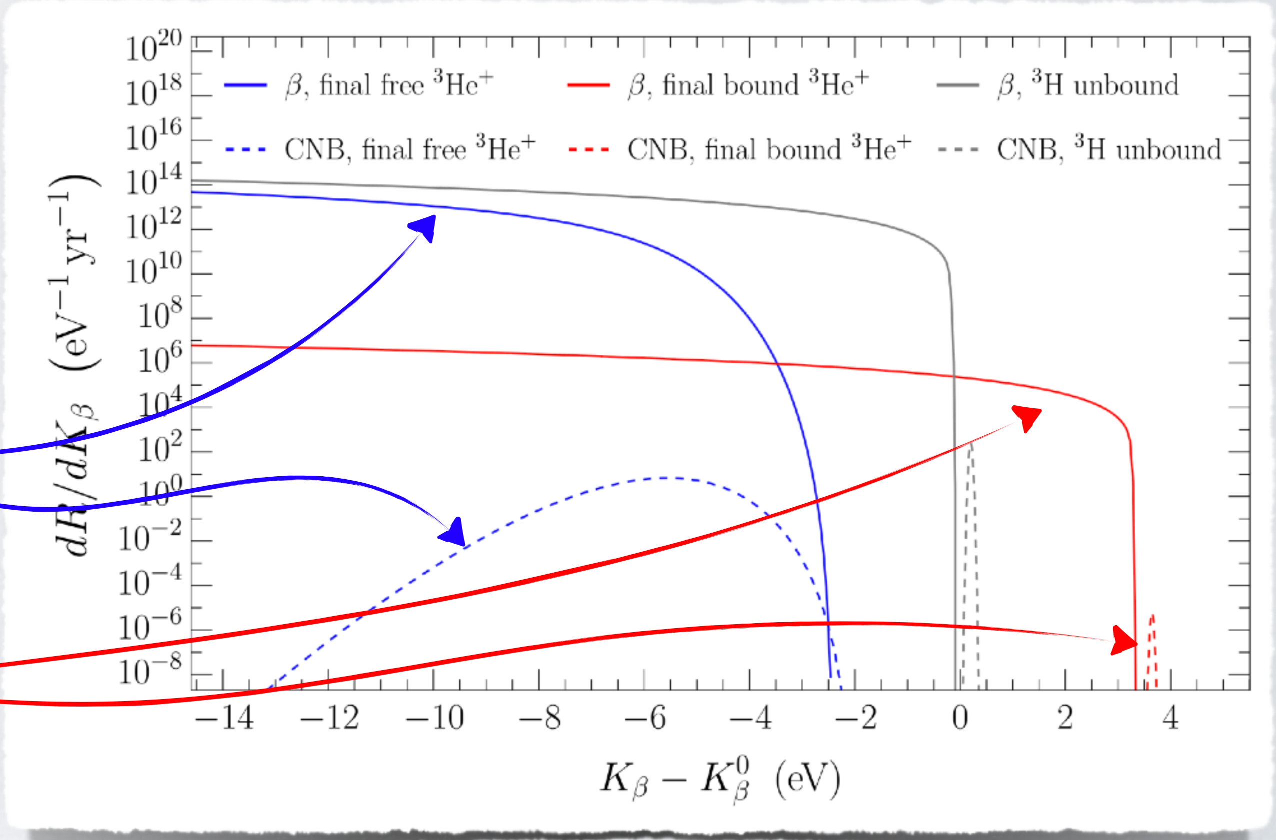
[Cheipesh, Cheianov, Boyarsky — PRD 2021, 2101.10069; Nussinov, Nussinov — PRD 2022, 2108.03695; PTOLEMY — PRD 2022, 2203.11228]

- Full quantum mechanical calculation:

[PTOLEMY — PRD 2022, 2203.11228]

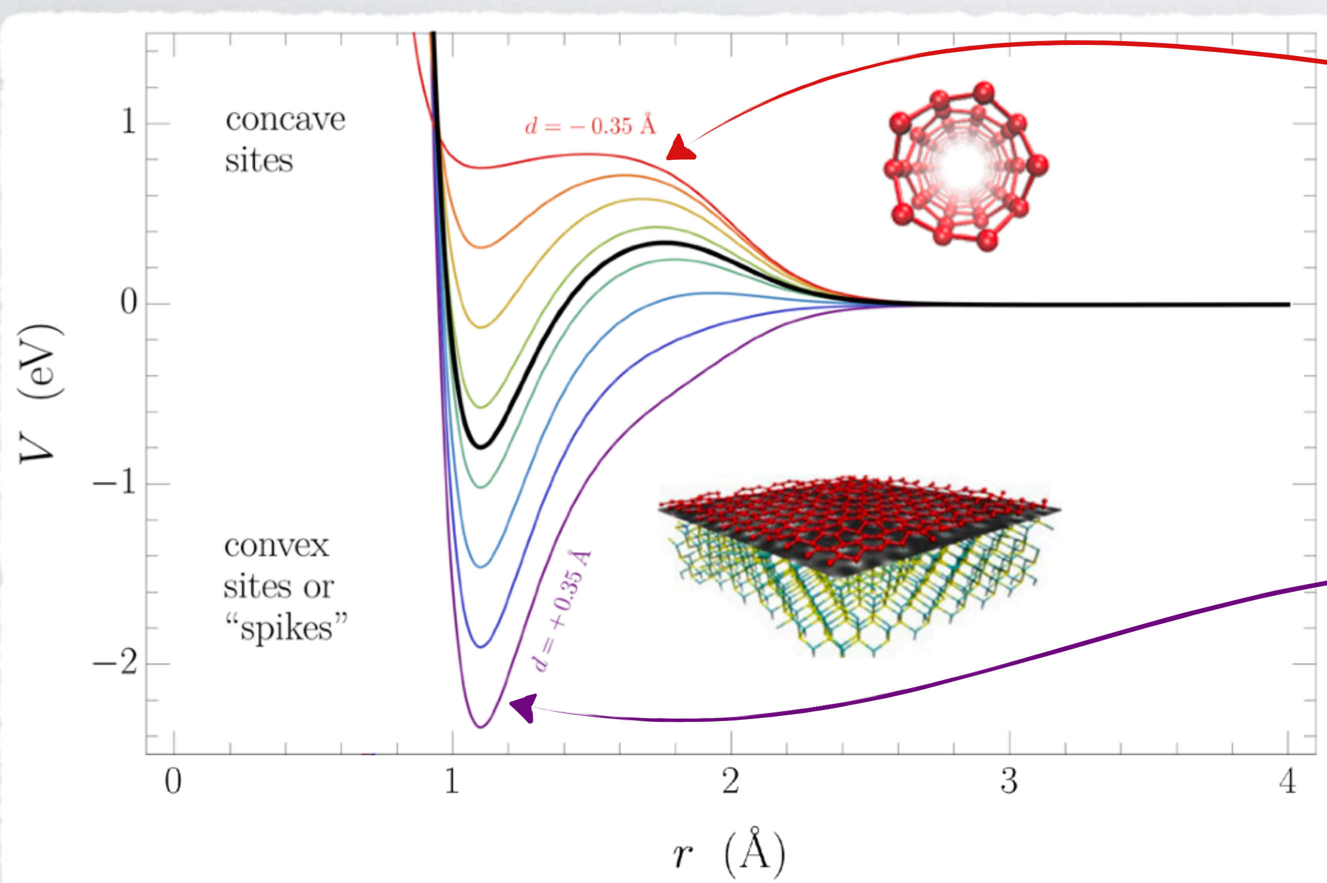
^{3}He$^+$ is freed from graphene $\longrightarrow$ most likely event but affected by quantum spread

^{3}He$^+$ remains in the ground state $\longrightarrow$ no spread but exponentially unlikely

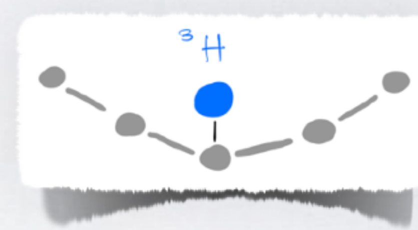


WHAT SUBSTRATE?

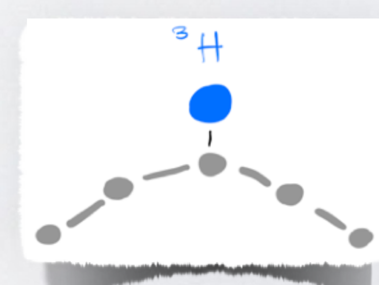
- Mitigate quantum effects from initially bound tritium → change binding potential → judicious tuning of the hosting material
- Potential for tritium on graphene depends on the local geometry



^3H on local concavity → **much shallower potential!**



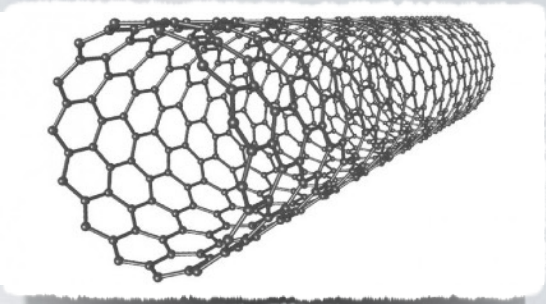
^3H on local convexity → deeper and more confining



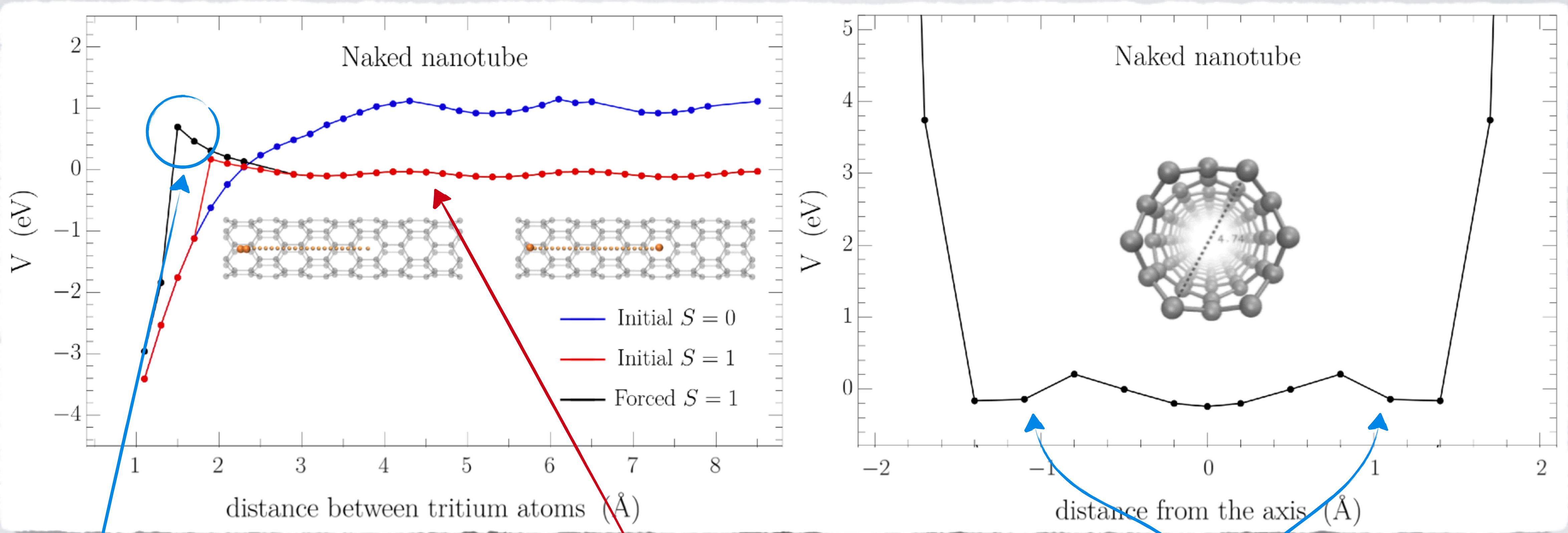
[PTOLEMY - PRD 2022, 2203.11228]

CARBON NANOTUBES

- Substrate with large concavity? → Nanotubes



- The tritium potential inside a nanotube is [PTOLEMY — PRD 2022, 2203.11228]



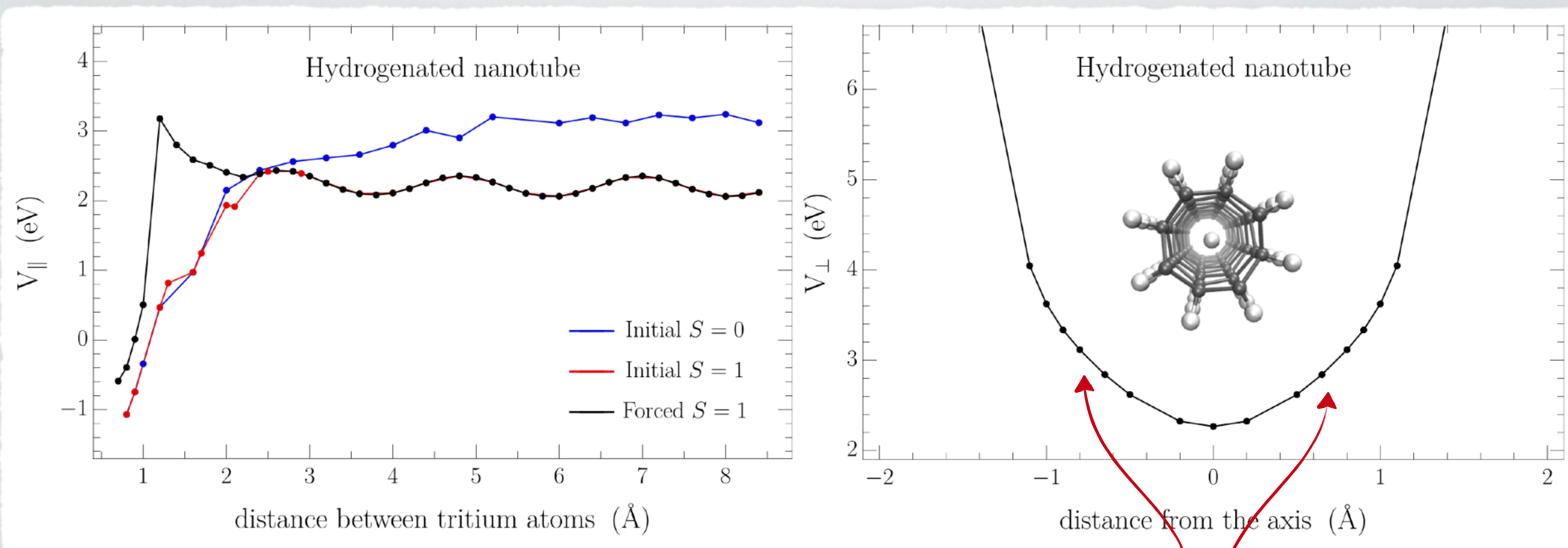
external $\boldsymbol{B}$ field can prevent formation of molecules

nicely flat

…but tritium can stick to the walls

CARBON NANOTUBES

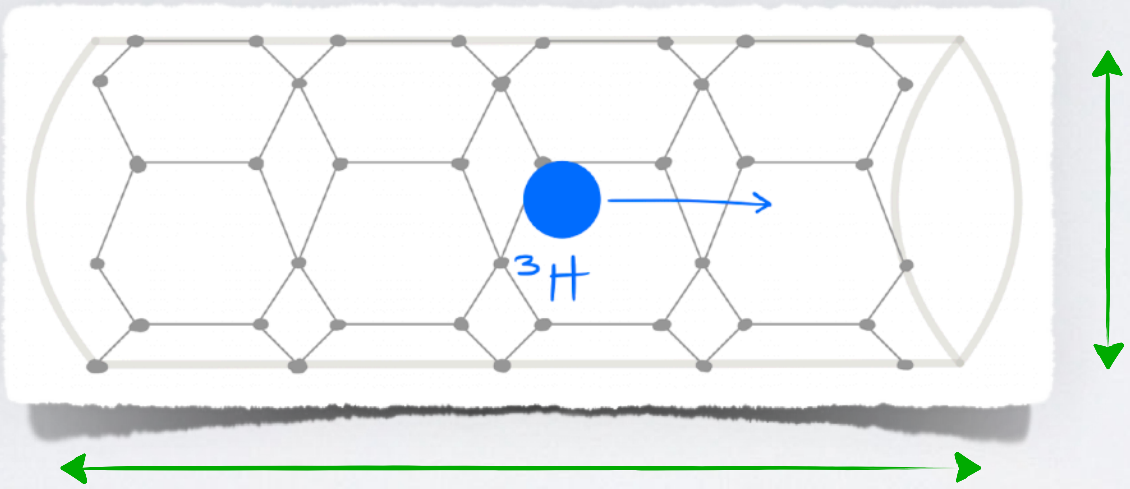
- To avoid sticky walls one can passivate the nanotube with hydrogen
- The new potential is [PTOLEMY – PRD 2022, 2203.11228]



two extra minima are now gone

CARBON NANOTUBES

- Ideally carbon nanotubes realize the following



- Assuming tightest packing without the formation of T_2 molecules one gets optimistically $10 - 20$ g of ^{3}H per kg of nanotubes
- A factor of 10 less than fully loaded graphene

CARBON NANOTUBES

- Aspects to be addressed:

A. What's the $\boldsymbol{B}$ field necessary to prevent dimerization? Is it compatible with PTOLEMY's needs?

B. How much tritium can we realistically store in nanotubes?

C. How do we grow and load the nanotubes according to our needs?

OTHER IDEAS?

- We want to delocalize the tritium $\rightarrow$ but not overshoot

- How delocalized should the tritium be?

$$\Delta E_e \sim \frac{p_e}{m_{He}} \frac{1}{\Delta x_T} = 0.05 \text{ eV} \qquad \Longrightarrow \qquad \Delta x_T \sim 2 \text{ Å}$$

- Might not be that much

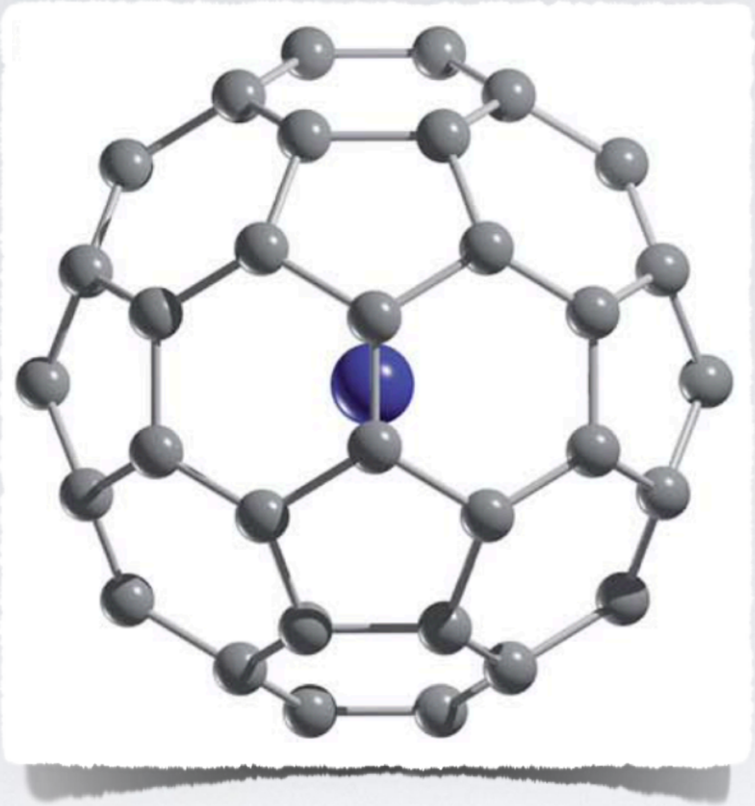
- Can we find a substrate that confines the tritium in a radius of around 2 Å?

FULLERENES

- A proposal is that of using fullerenes

[see, e.g., Guo et al. — Nature 1991; Frapiccini, Mitnik — EPJD 2021, 2010.15050; Deshmukh et al. — EPJD 2021]

^{3}H confined in the center



C_{60} – fcc

Lattice spacing is $a \simeq 14.3$ Å and a cubic cell contains 4 atoms

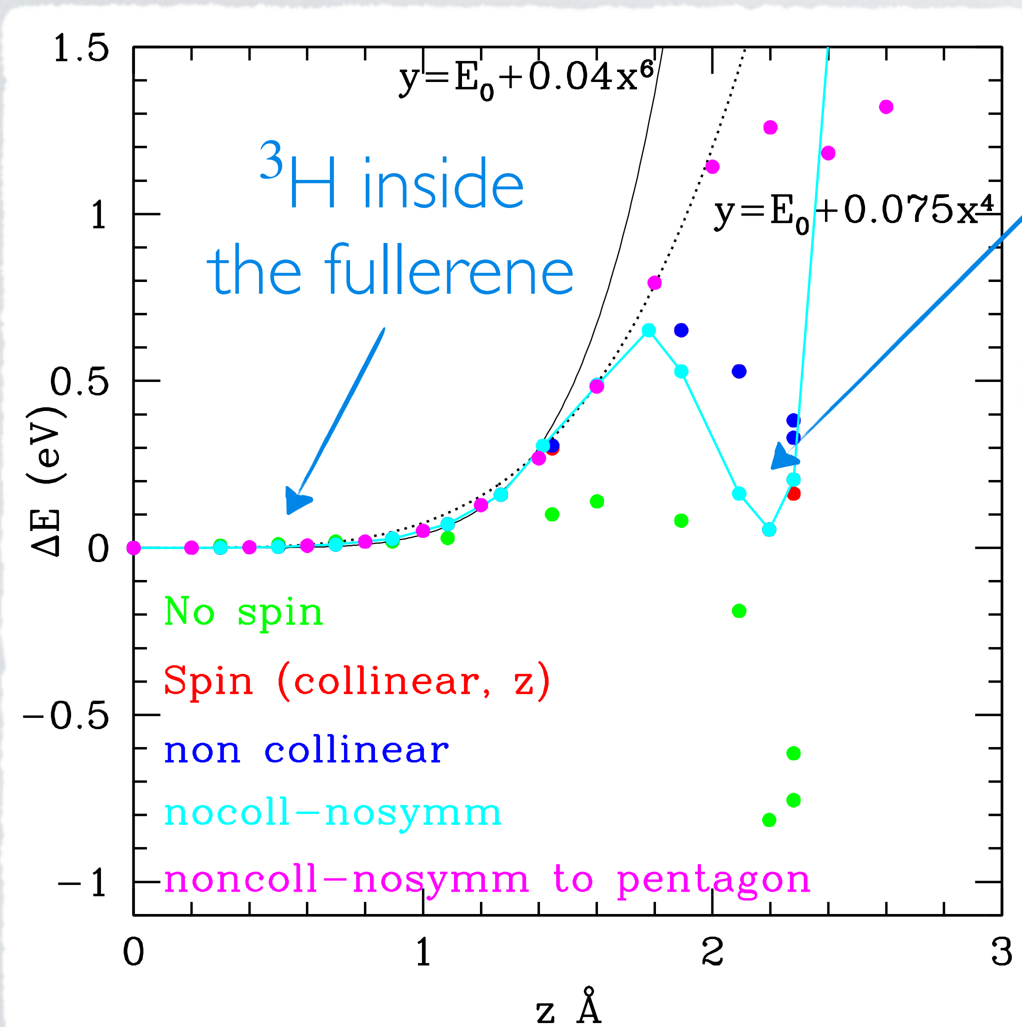
⇩

possible density of tritium $\rho_T \simeq 6.8$ mg/cm^3

- Seems like a possible ideal middle ground

FULLERENES

- Preliminary ab initio calculations for a naked isolated fullerene give (see Valentina's talk!)



^{3}H sticks to the wall

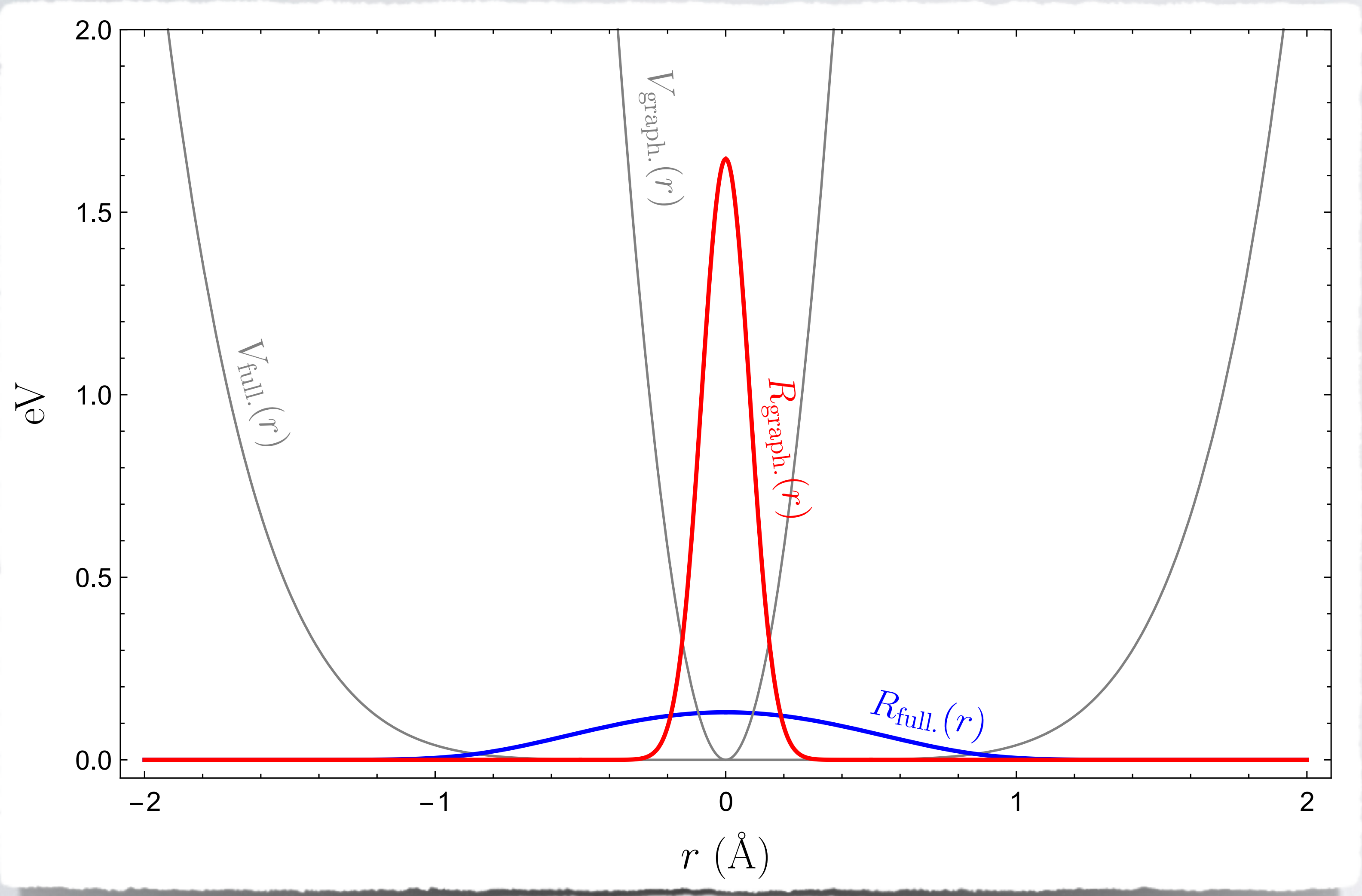
Potential in the center is well approximated by

$$V(r) \simeq \left(0.04\ \mathrm{eV}/\mathrm{Å}^6\right) r^6$$

What consequences for us?

FULLERENES

- Wave function of tritium at the center of a fullerenes



Fullerenes do better than graphene already

From the wave function we find

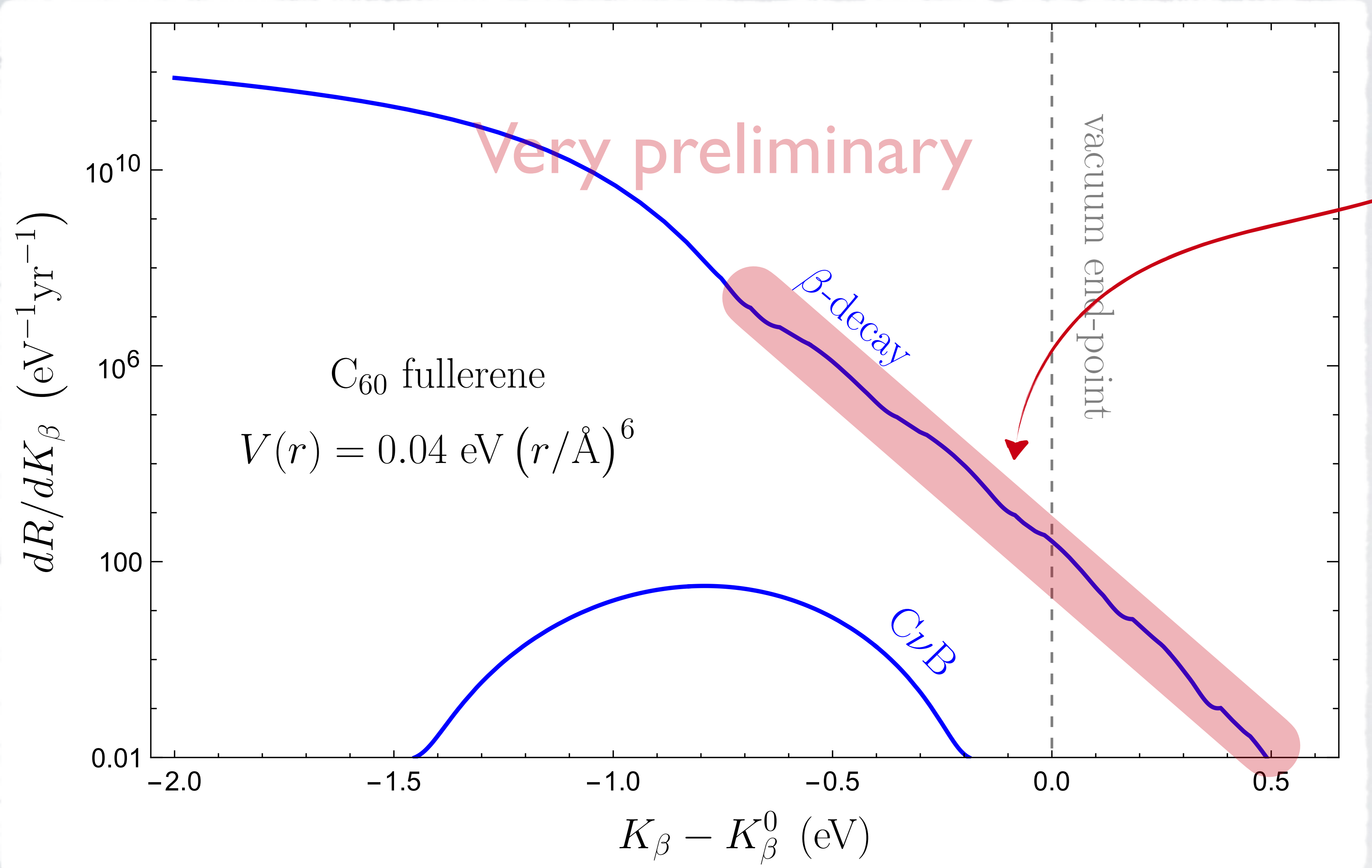
$$\Delta x_T \simeq 0.29\ \text{Å}$$

$$\Delta p_T \simeq 3.4\ \text{keV}$$

$$\Delta K_e \simeq 0.17\ \text{eV}$$

FULLERENES

- (Very) preliminary quantum calculation returns:



still working on this… ready soon!

FULLERENES

- I suck at numerics, but… some things to understand about fullerenes:

  A. What is the exact potential? → include many cells in a crystal, compute for a hydrogenated structure, bigger cells, …

  B. How much tritium can we load on it?

  C. How do we do it?

- Stay tuned!

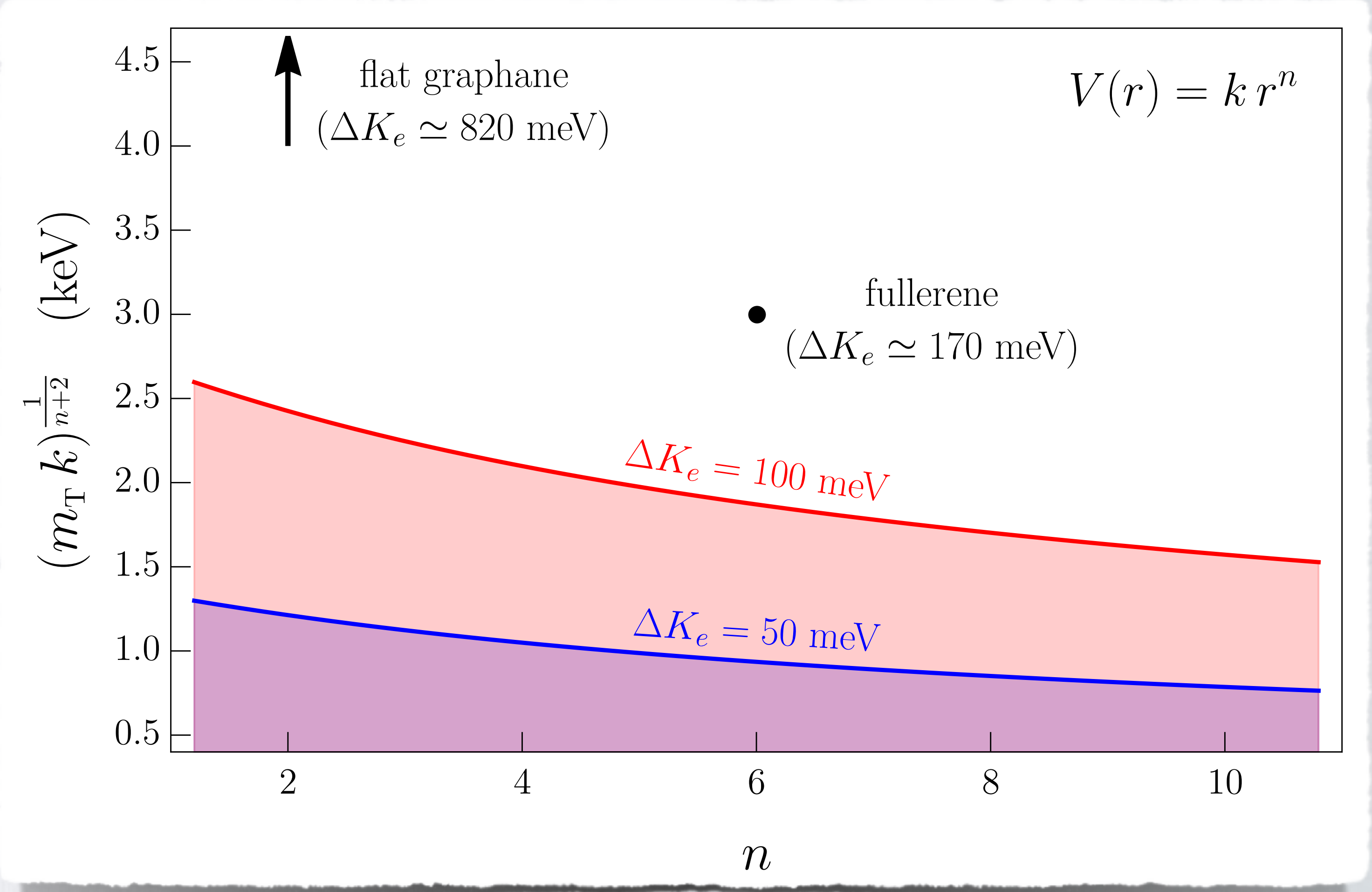
WISHLIST

- For a binding potential $V(r) = k\,r^n$ the momentum uncertainty roughly follow the empirical formula:

$$\Delta p_T(k,n) \simeq \frac{\sqrt{\frac{n}{2}+1}}{2}\,(2m_T k)^{\frac{1}{n+2}}$$

(good up to $n \simeq 10$)

- What we want from Santa this year:



OUTLOOK

- PTOLEMY's goal is an ambitious one → worth the effort!
- Storing ^{3}H on a solid has great advantages… but also raises issues
- If we stick to ^{3}H, the solution to the problem of intrinsic uncertainty must come from a judicious choice of the host material
- Quoting Alexey, also several other effects to be understood and taken into account

Thank you for your attention!