Hydrogenation of CNTs

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Motivation

First results

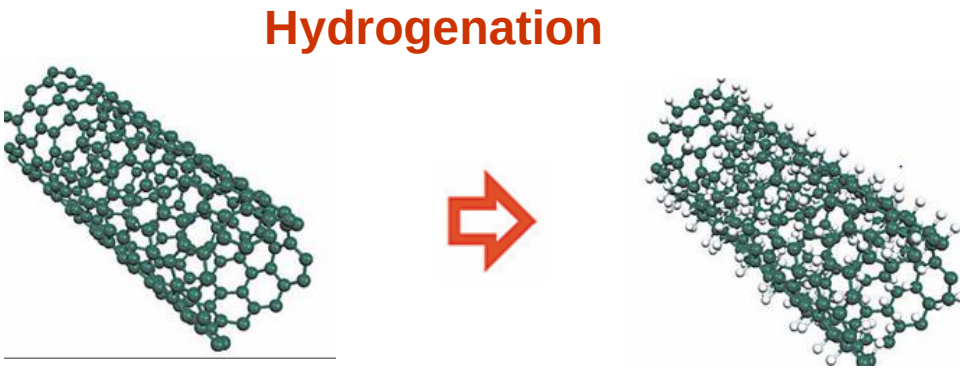
Perspectives

- scientific motivation: H, D towards T chemisorption on sp2-bonded C atom meshes → sp3 bonds

- exploited so far different atomic H (D) deposition methods:
  (i) plasma (it damages the mesh);
  (ii) low-energy ions (high uptake and less damage);
  (iii) ≤0.2 eV atoms (very high uptake and no damage)

- previous results of (iii) on nanoporous free-standing graphene (NPGr) ~90%* and on flat Gr ~100%** uptake (see Roma Tre experiments)

- how does H-uptake uptake change on nm-curved Gr surfaces (CNTs)?

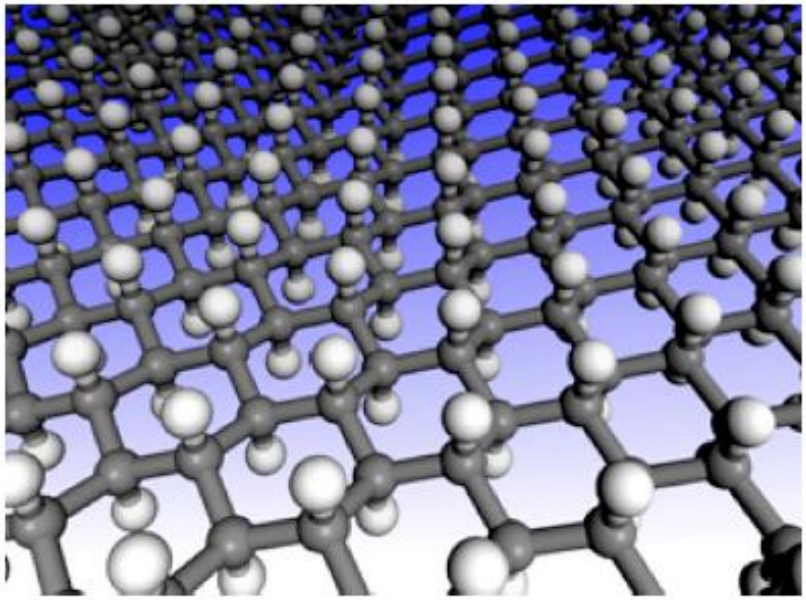


* Betti et al., Nano Lett. **22**, 2971 (2022); ** Ruocco et al., to be published

from graphene to graphane, theory

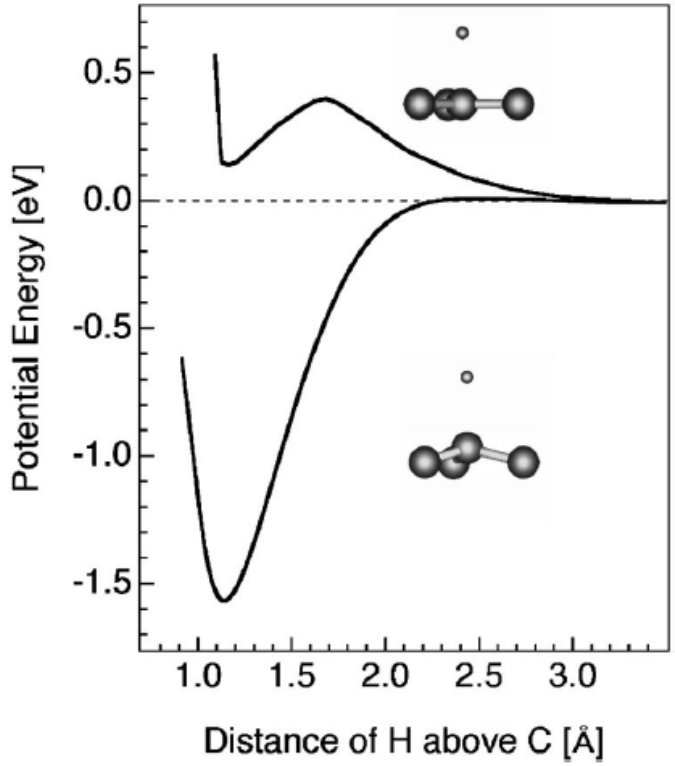
atomic H as a tool to '*pinch*' the sp2 bonds towards an sp3 configuration while maintaining the planar nature of graphene

"chair" conformation



Sofo et alii, Phys. Rev. B **75**, 153401 (2007)

covalent bonding, small charge transfer (~0.003 e)*

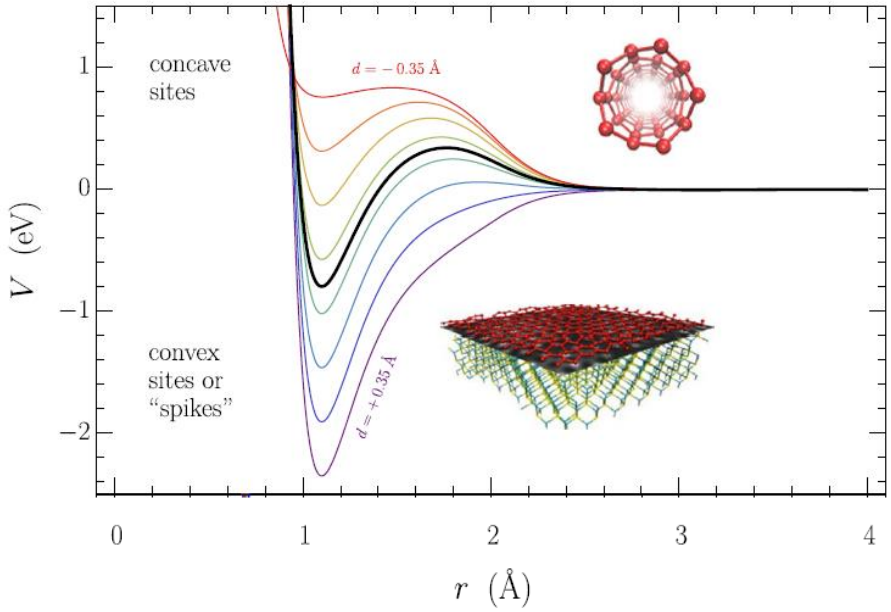


H-to-C potential curve -> favoured sp3 configuration

Ryu et alii, Nano Lett. **8**, 4597 (2008)

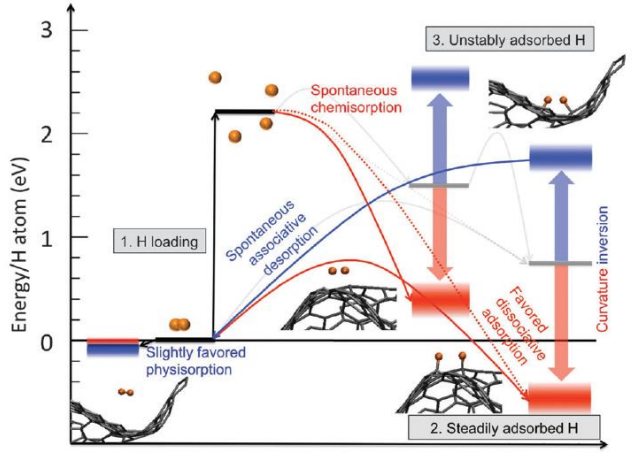
Ruffieux et alii, Phys. Rev. B **66**, 245416 (2002)

from graphene to graphane, theory

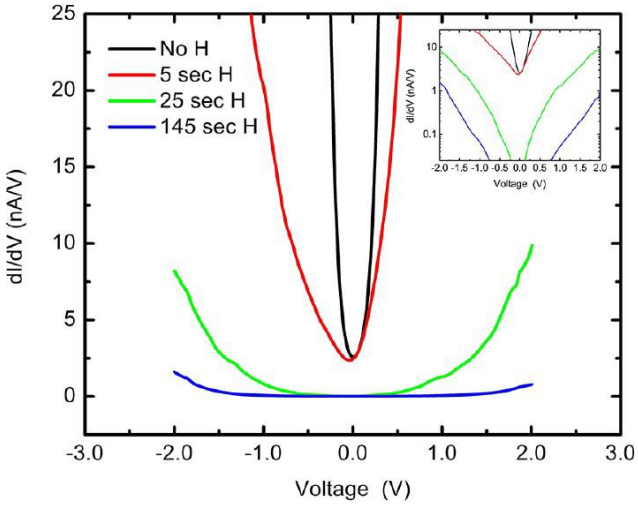


Apponi et al. (Ptolemy), Phys. Rev. D **106**, 053002 (2022)

convexity (with respect to graphene plane) **lowers H-C chemisorption energy barrier**



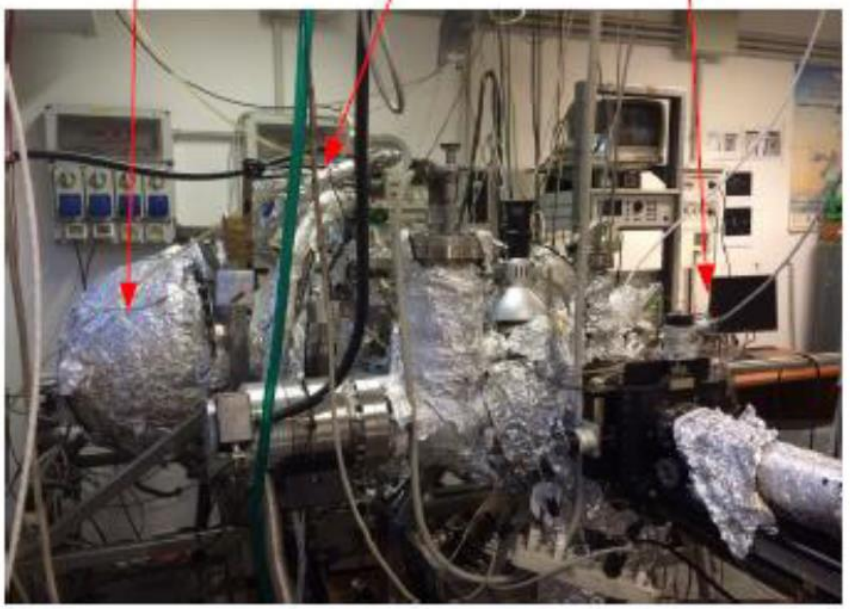
Tozzini and Pellegrini, Phys. Chem. Chem. Phys. **15**, 80 (2013)

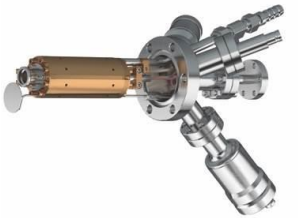


Goler et al., J. Phys. Chem. **117**, 11506 (2013)

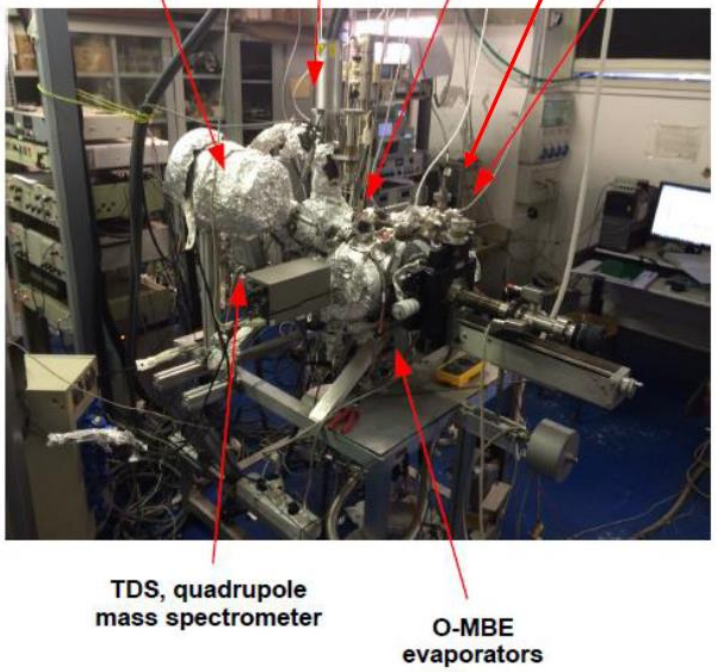
← experimental STS shows an **energy gap** at **convex Gr** zones exposed to **H**

Nanostructures at Surfaces Laboratory @ Sapienza

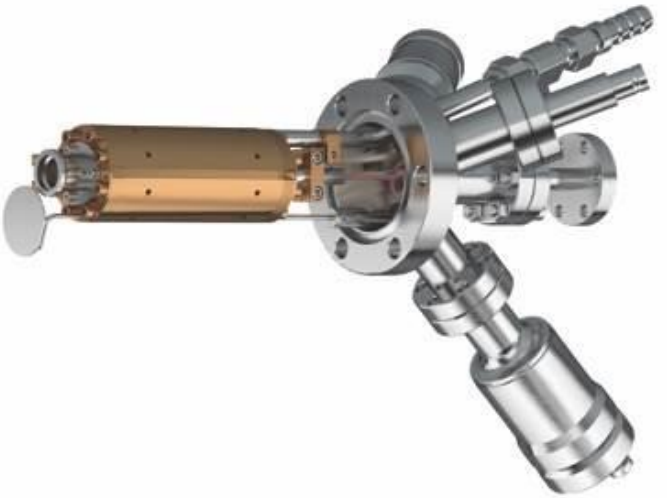


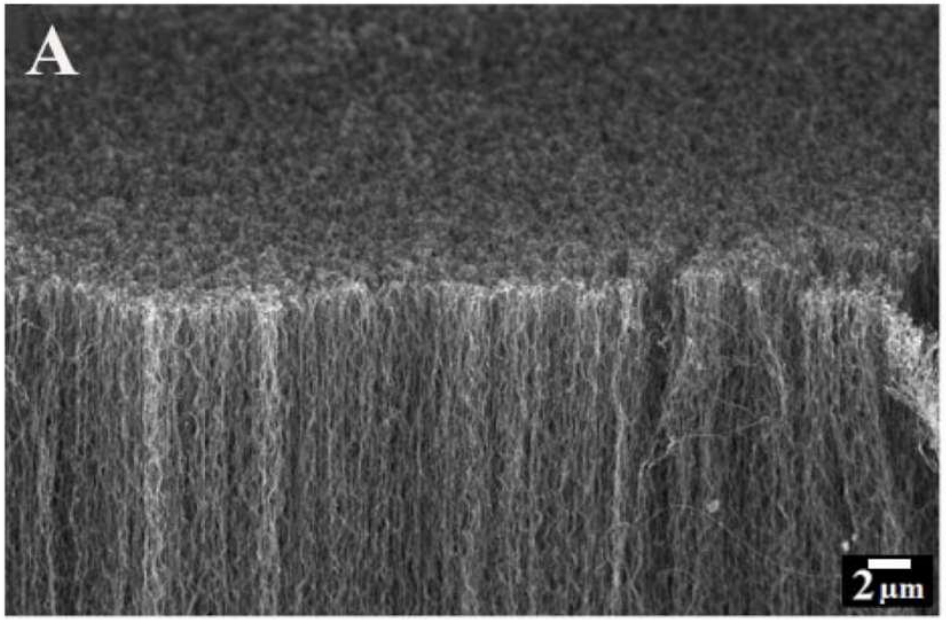


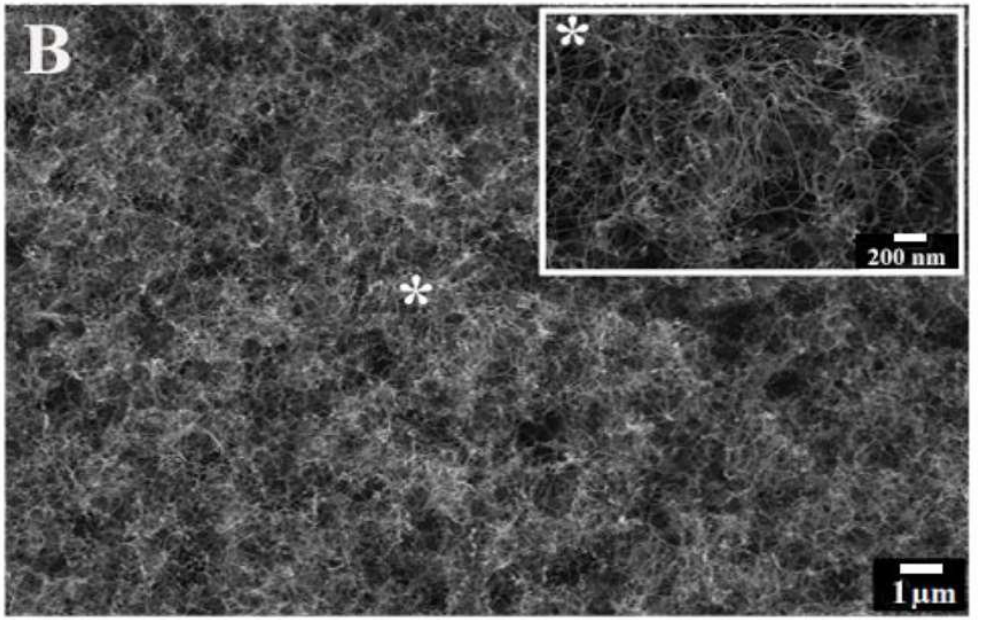
atomic H source



https://sites.google.com/uniroma1.it/nano-surface-physics/home





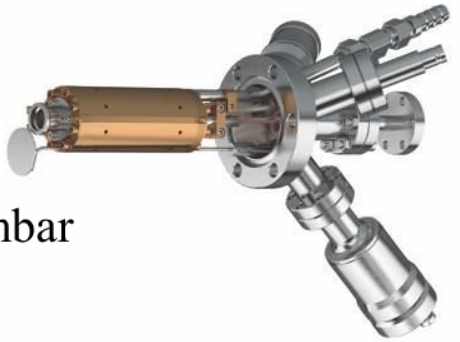


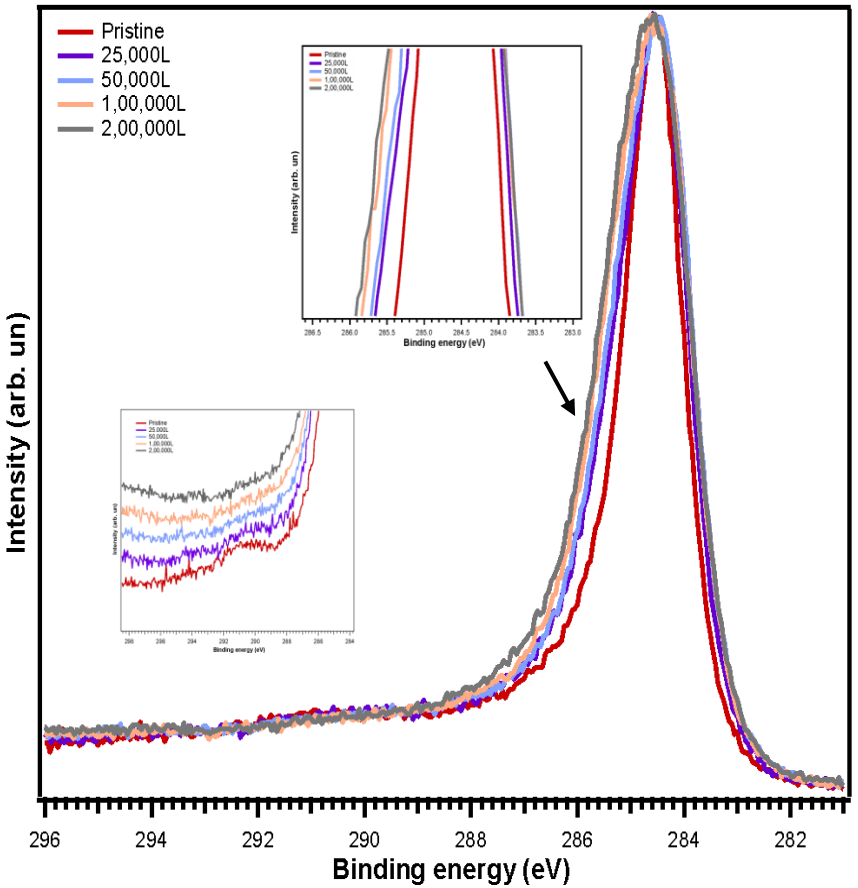
Ilaria Rago et al., INFN-Sapienza CVD facility for CNT growth

first measurements of atomic D chemisorption on MW-CNTs

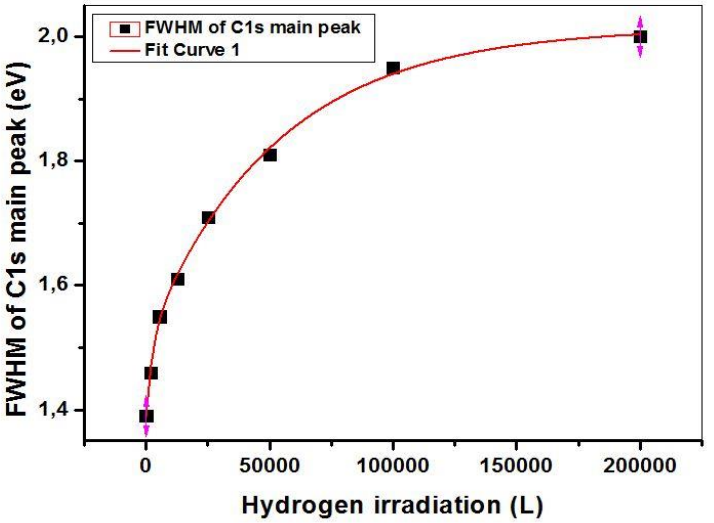
❑ **Parameters used to crack D_2 in UHV:**

Power = 6.5W; capillary T= 1400K; p=1×10^{-6} mbar





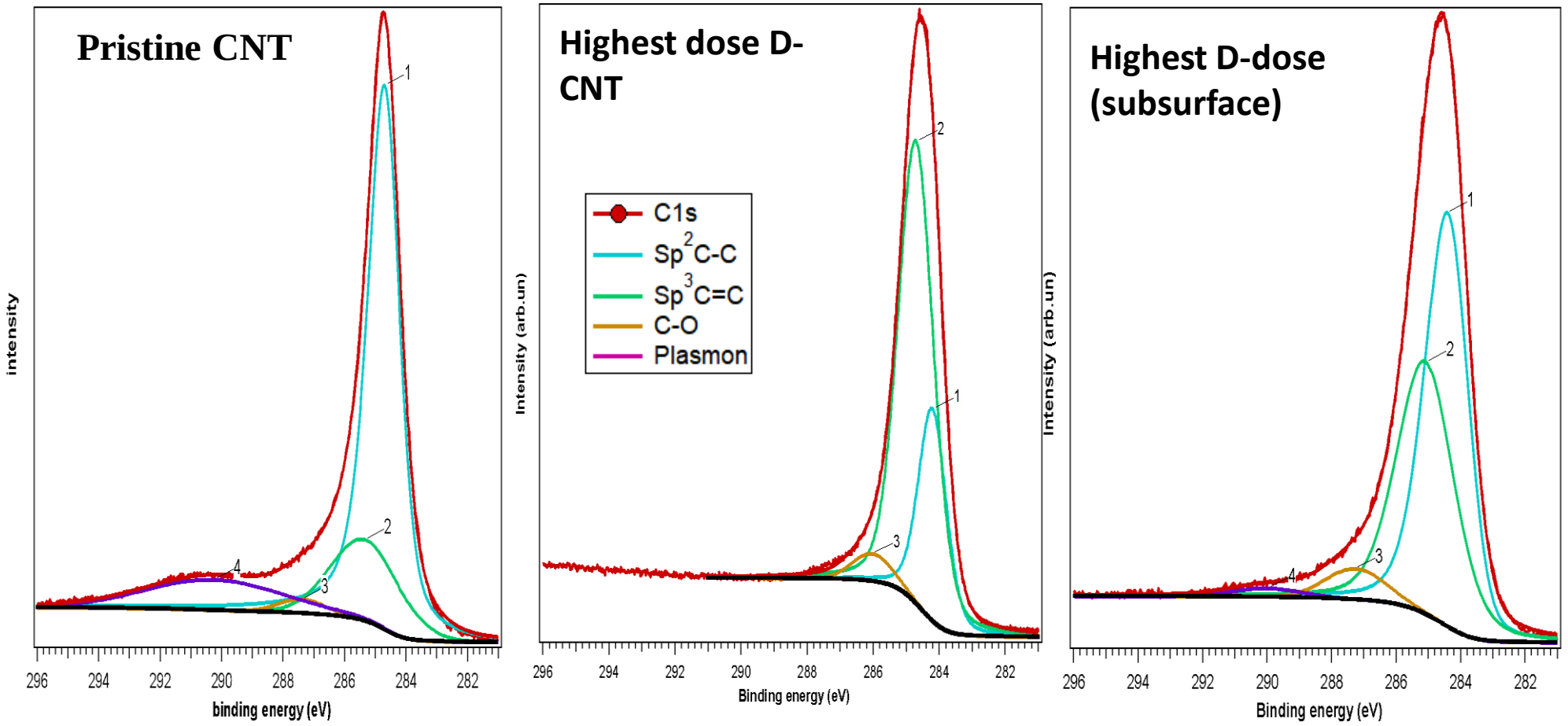
XPS measurements of C 1s core-level



Langmuir exposure unit

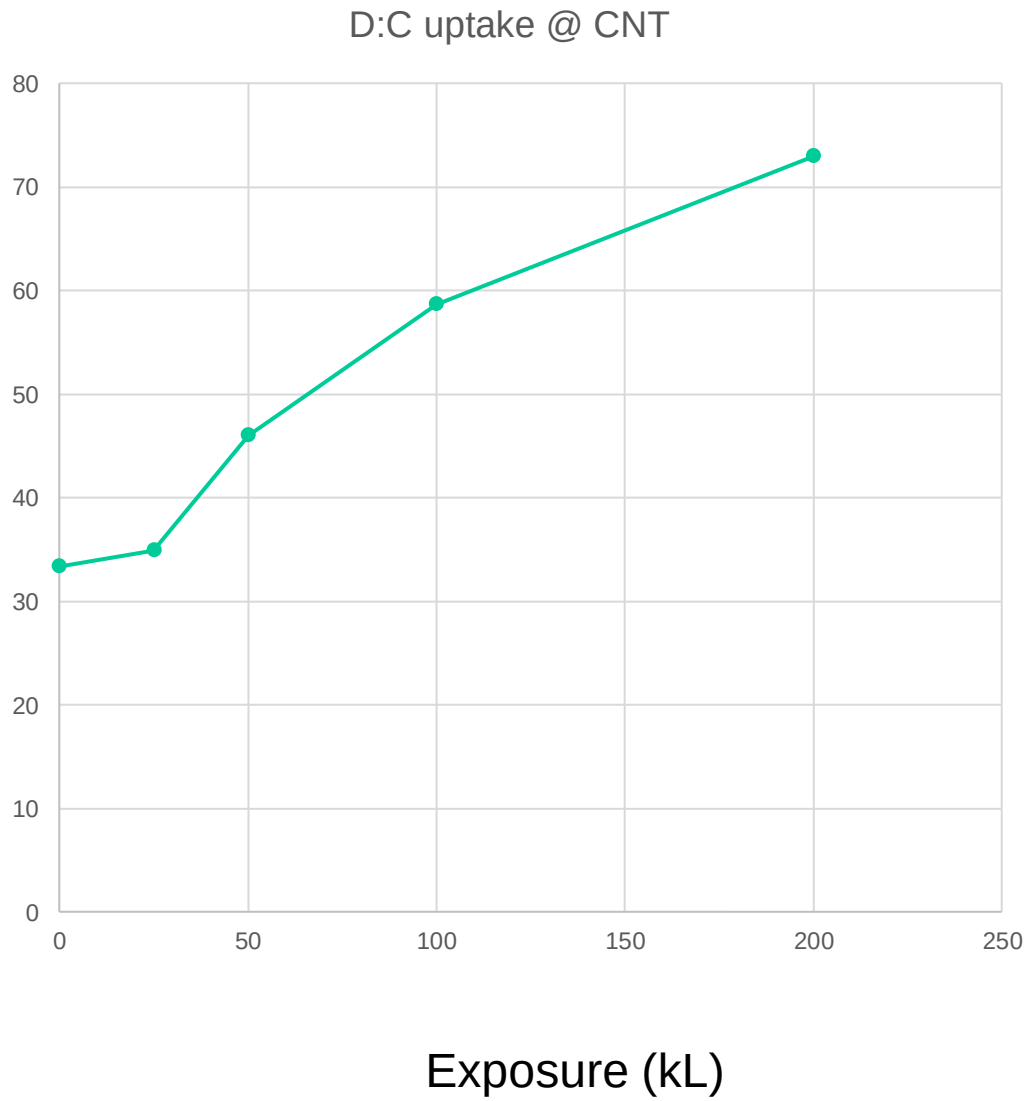
1 L = 1 sec *x* 10^{-6} torr

first results: evaluation of D:C uptake



	pristine CNT (±5%)		D-CNT (±5%)
atomic % D:C upload [sp3/(sp3+sp2)]	**21%**	→	**73% @ surface** (46% subsurface)
Δ BE	**0.5 eV**		

first results: evaluation of D:C uptake



perspectives

- **temperature stability evaluation of D-C bond**

- **crystal lattice characterization via Raman spectroscopy**

- **evaluation of (i) curvature vs. (ii) n. Gr layers for the saturation uptake → comparison with flat monolayer Gr, NPG**

- **further questions: interplay of alkali-metals and H uptake on CNTs**