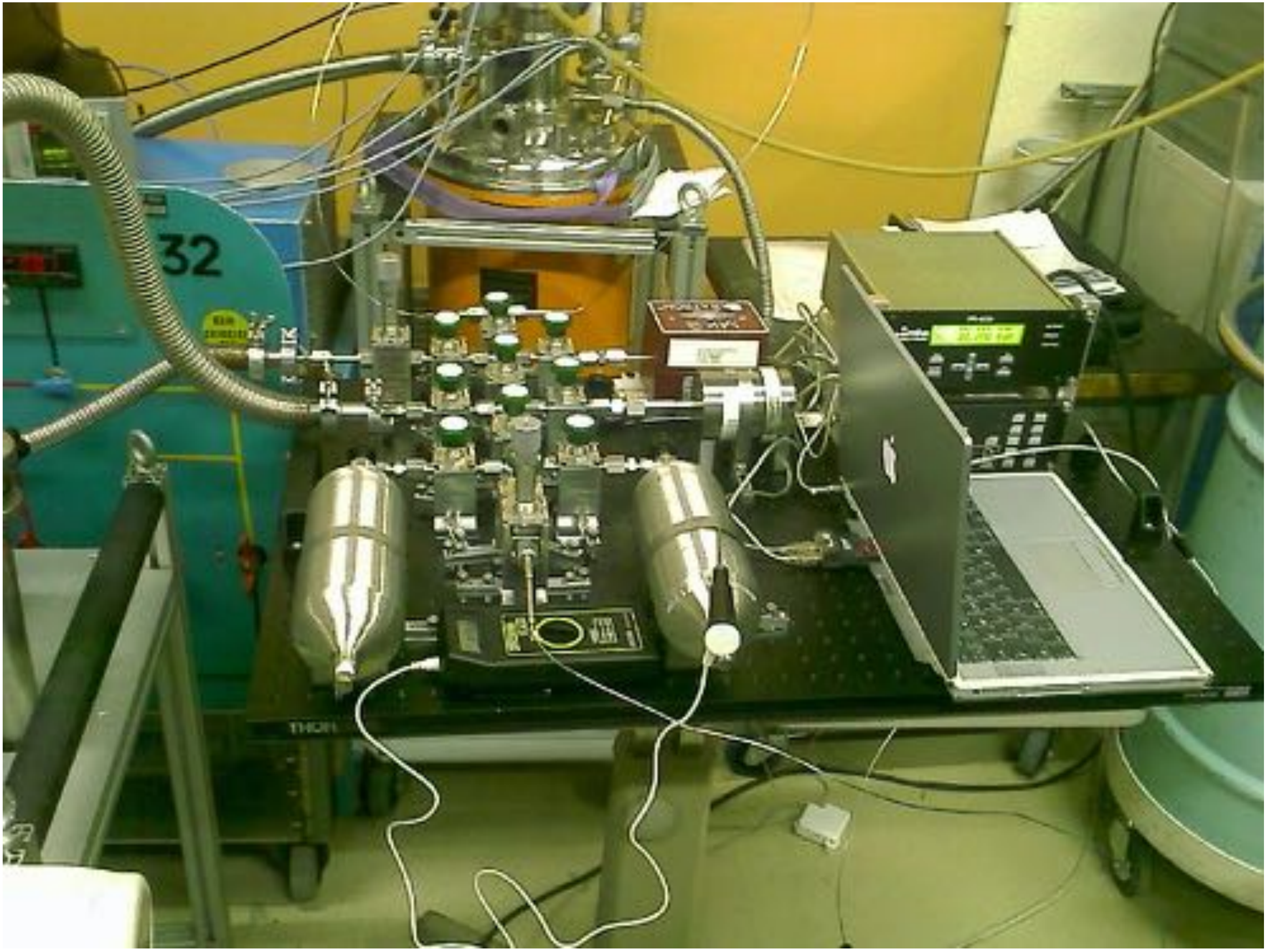
Entrevista con el grupo de investigación Sistemas Carentes de Orden de Largo Alcance

Dr. Carlos Cabrillo, 917040693
915616800 xtn 442297, Serrano 123,
Despacho 136
(ccabrilo@foton0.iem.csic.es)

Dr. Ricardo Fernández, 917040674
915616800 xtn 442276, Serrano 123,
Despacho 109
(ricardo@langran.iem.csic.es)

Dispersión de Neutrones

Dispersión de Neutrones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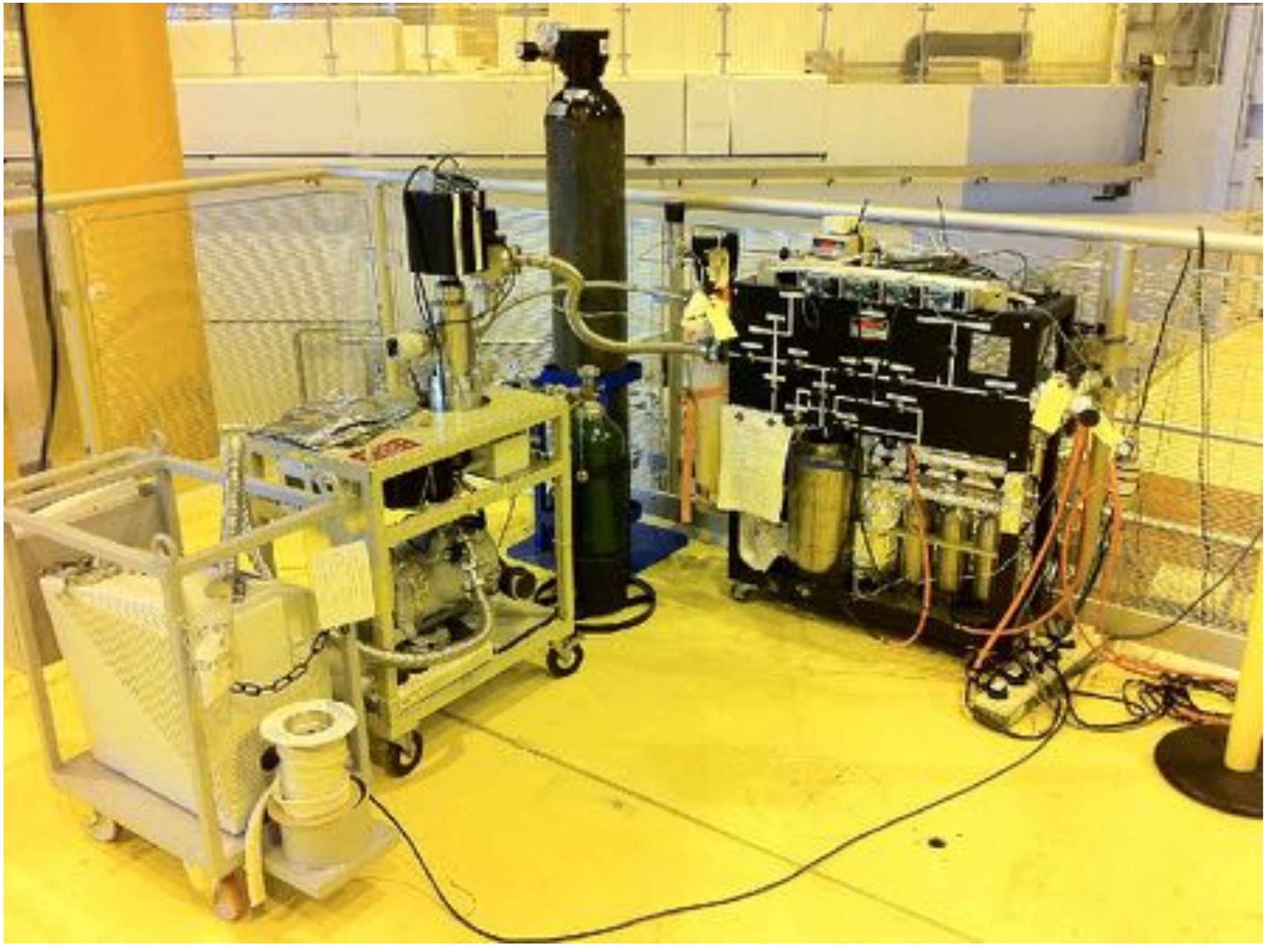
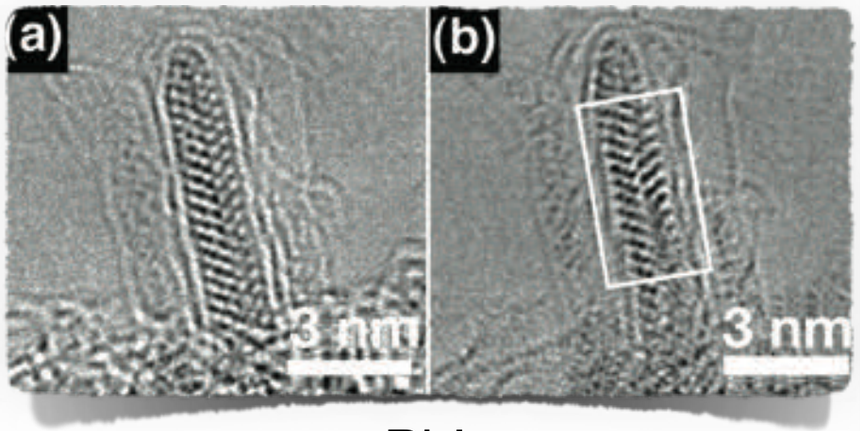


1D Crystallisation

E. Flahaut et al, *Chem. Mater.* 18, 2059 (2006)



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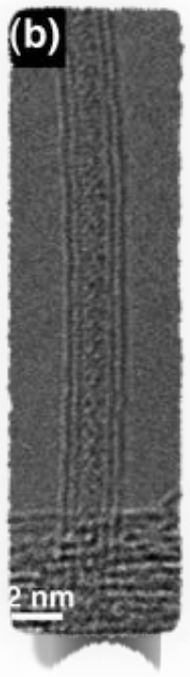
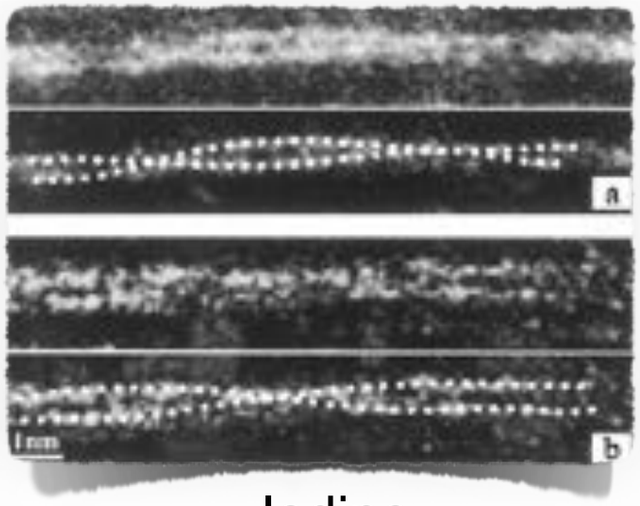
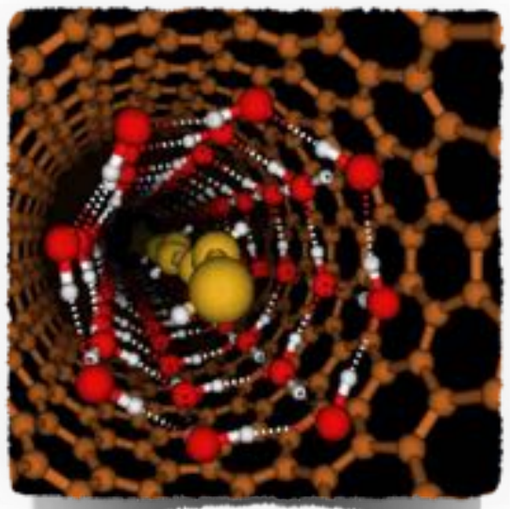


X. Fan et al., *Physical Review Letters* 84, 4621 (2000)



Iodine

A. I. Kolesnikov et al., *Physical Review Letters* 93, 035503 (2004)



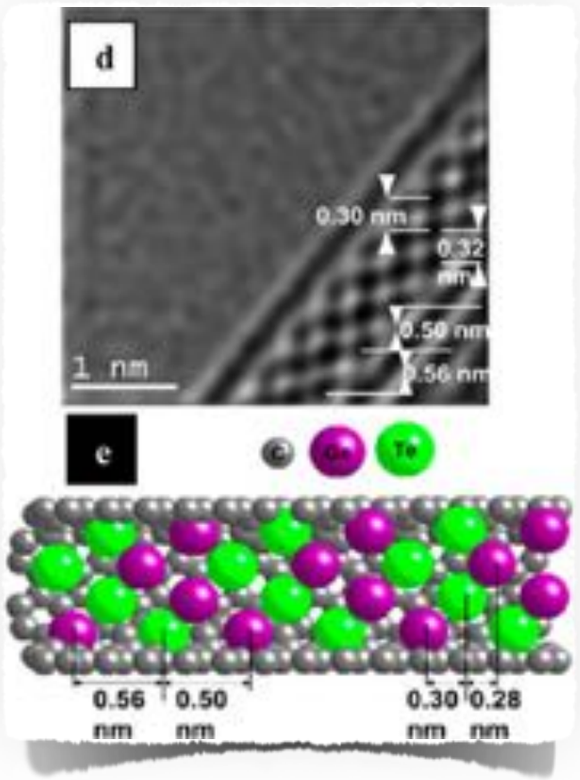
Water

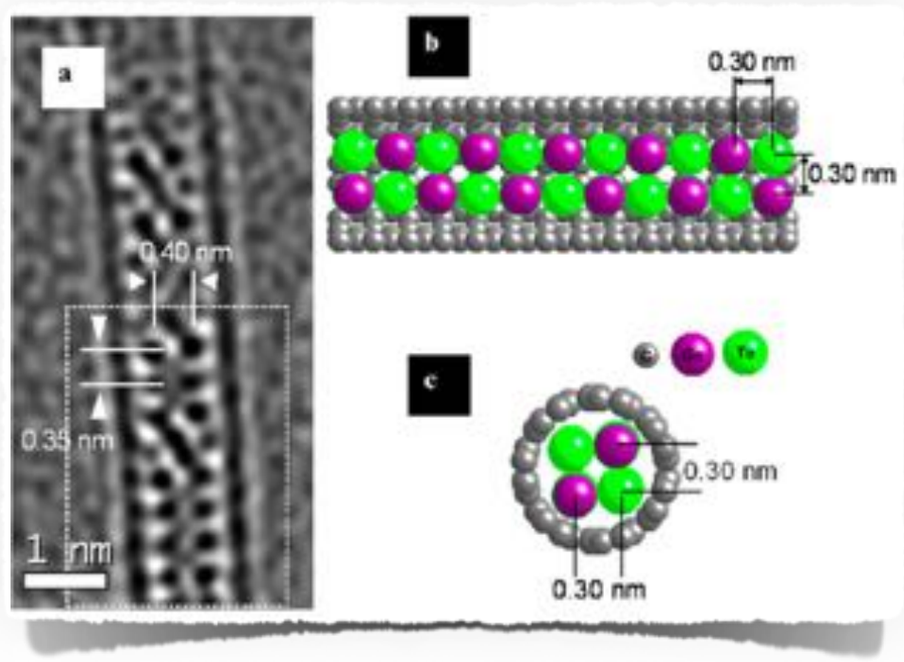
Cohesive interaction >> Adsorption interaction

GeTe

Strict 1D limit

Giusca, C. E. et al., *Nano letters* 13, 4020–4027 (2013).





1D Crystallisation

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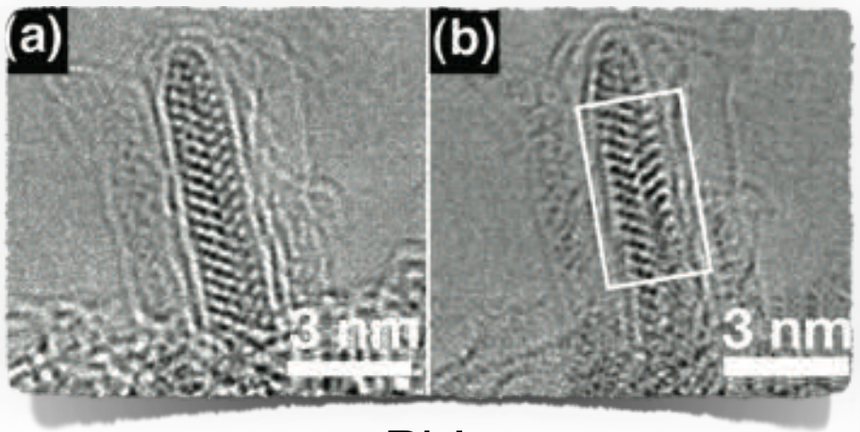

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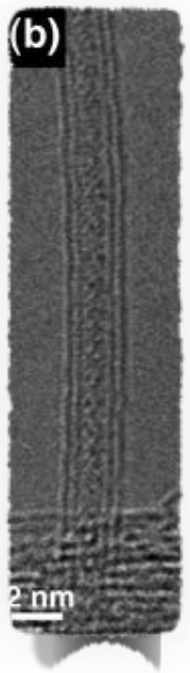

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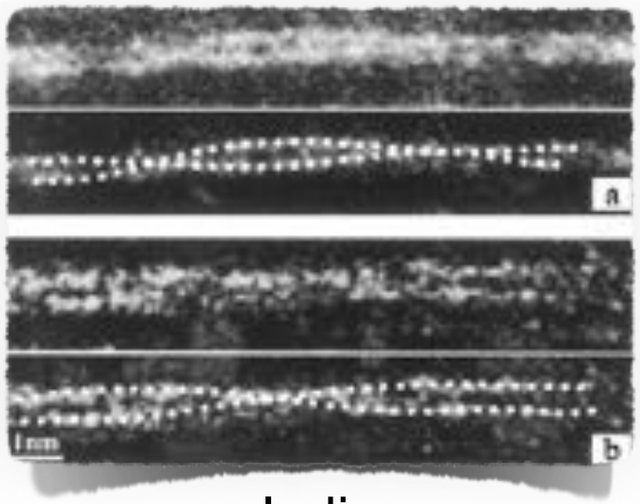
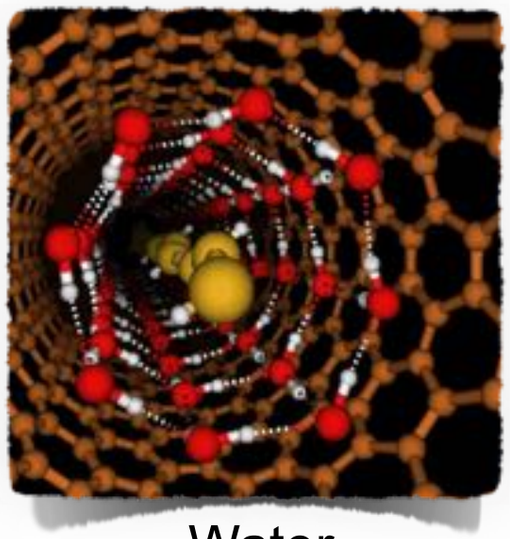


Iodine

A. I. Kolesnikov et al., *Physical Review Letters* 93, 035503 (2004)



Water

H_2

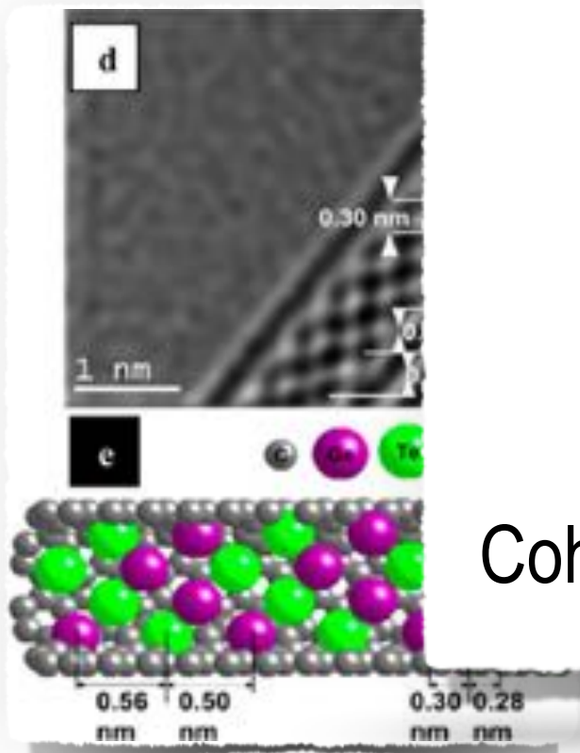
H_2 interaction potencial depth:

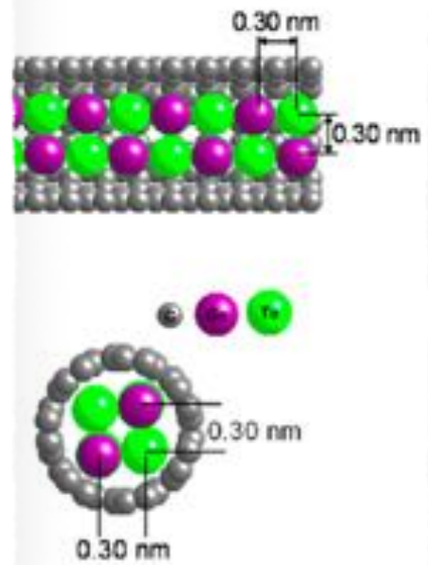
− 2.77 meV

Graphite adsorption potencial depth:

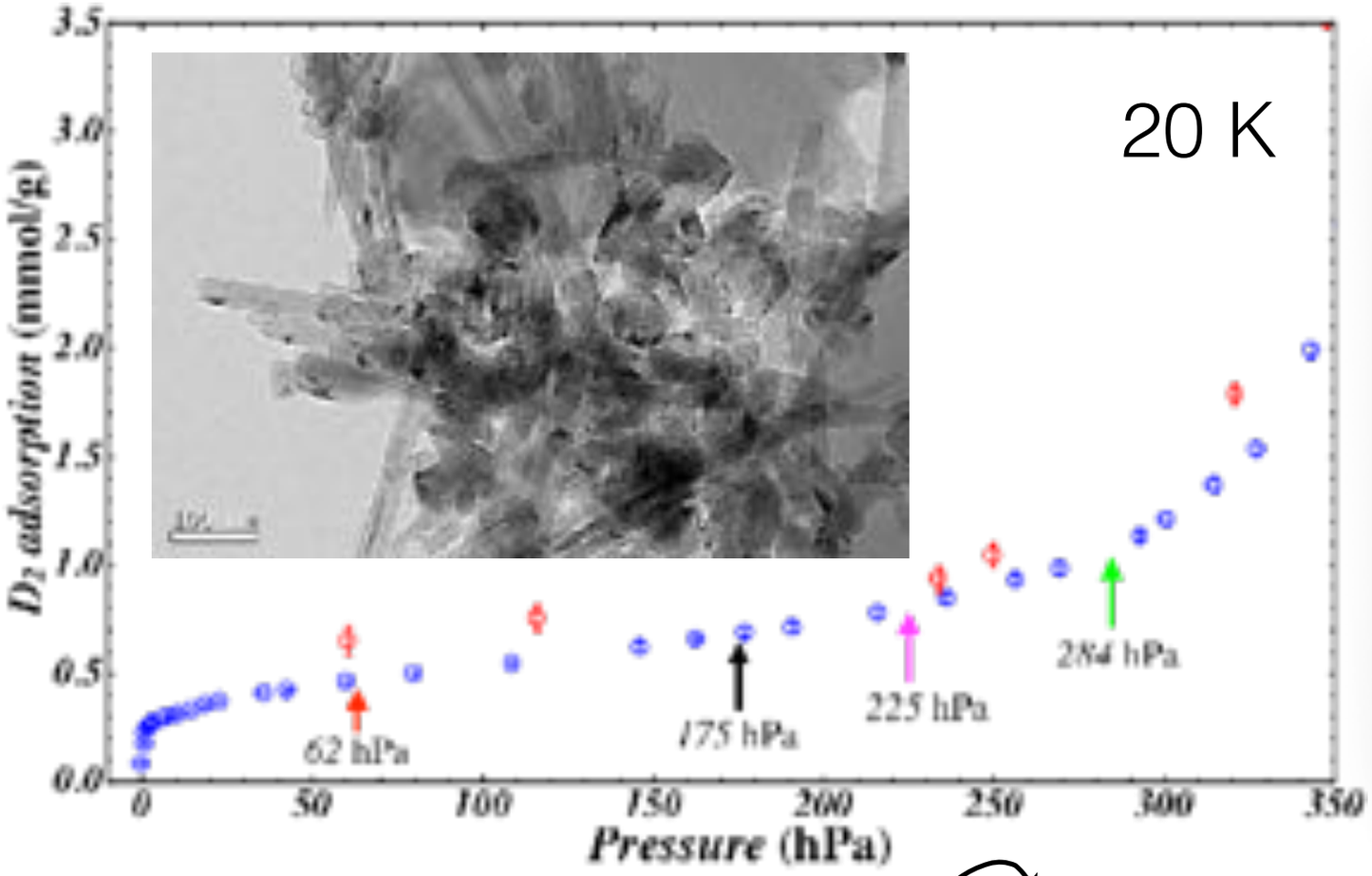
~ − 50 meV

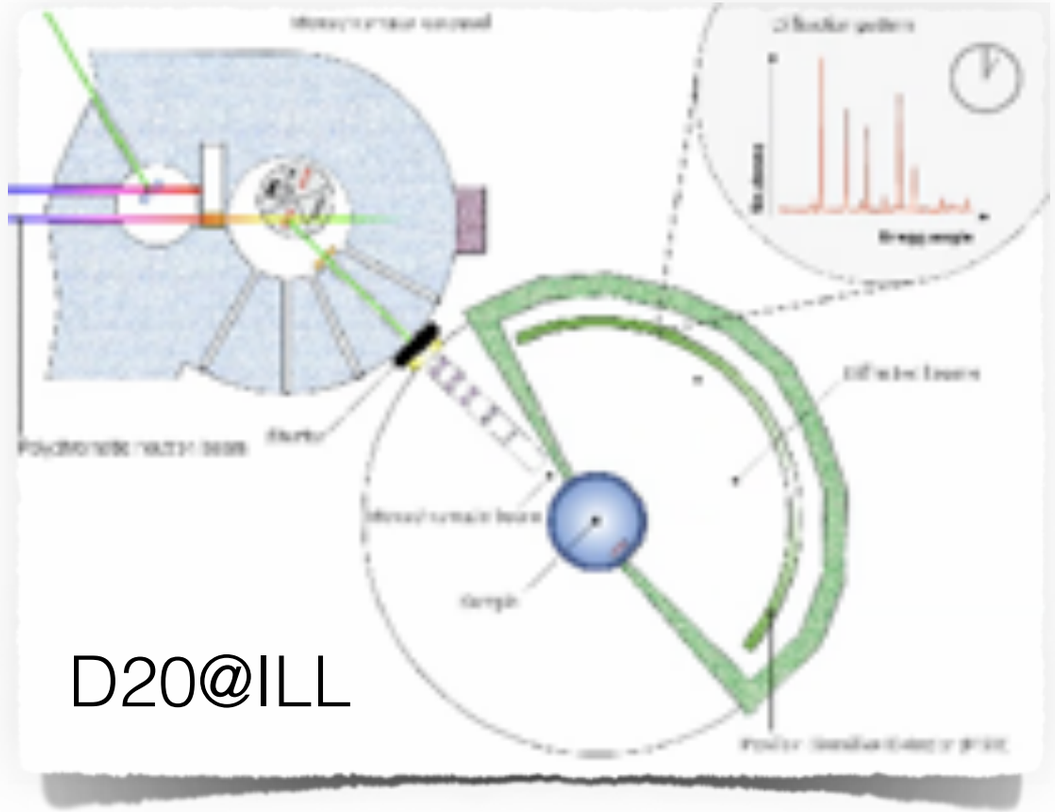
Cohesive interaction << Adsorption interaction

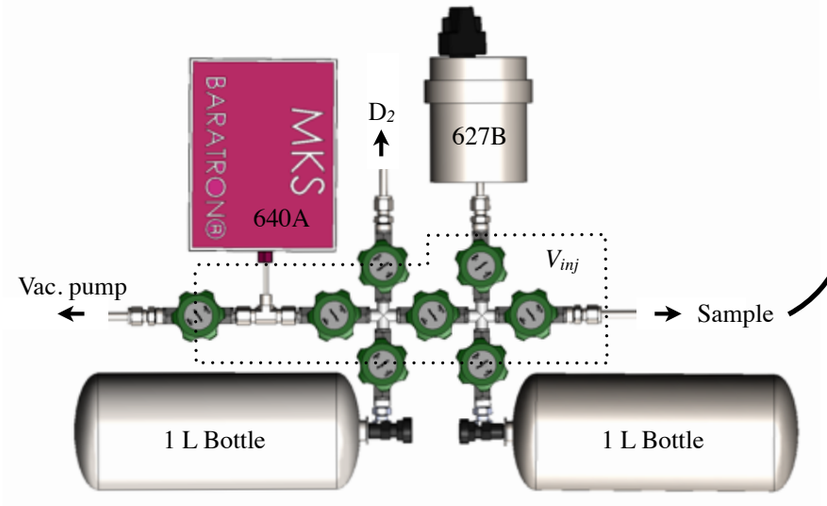


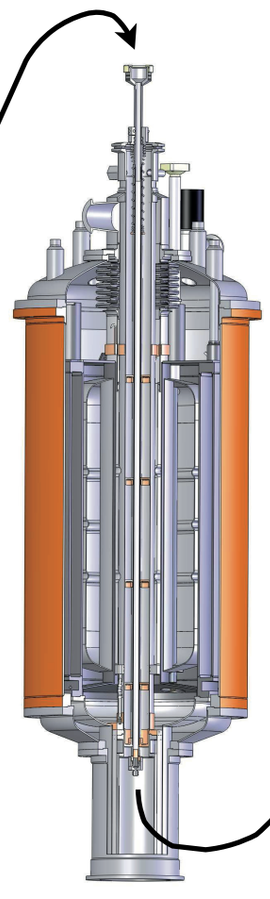


1D Crystallisation: our experiment





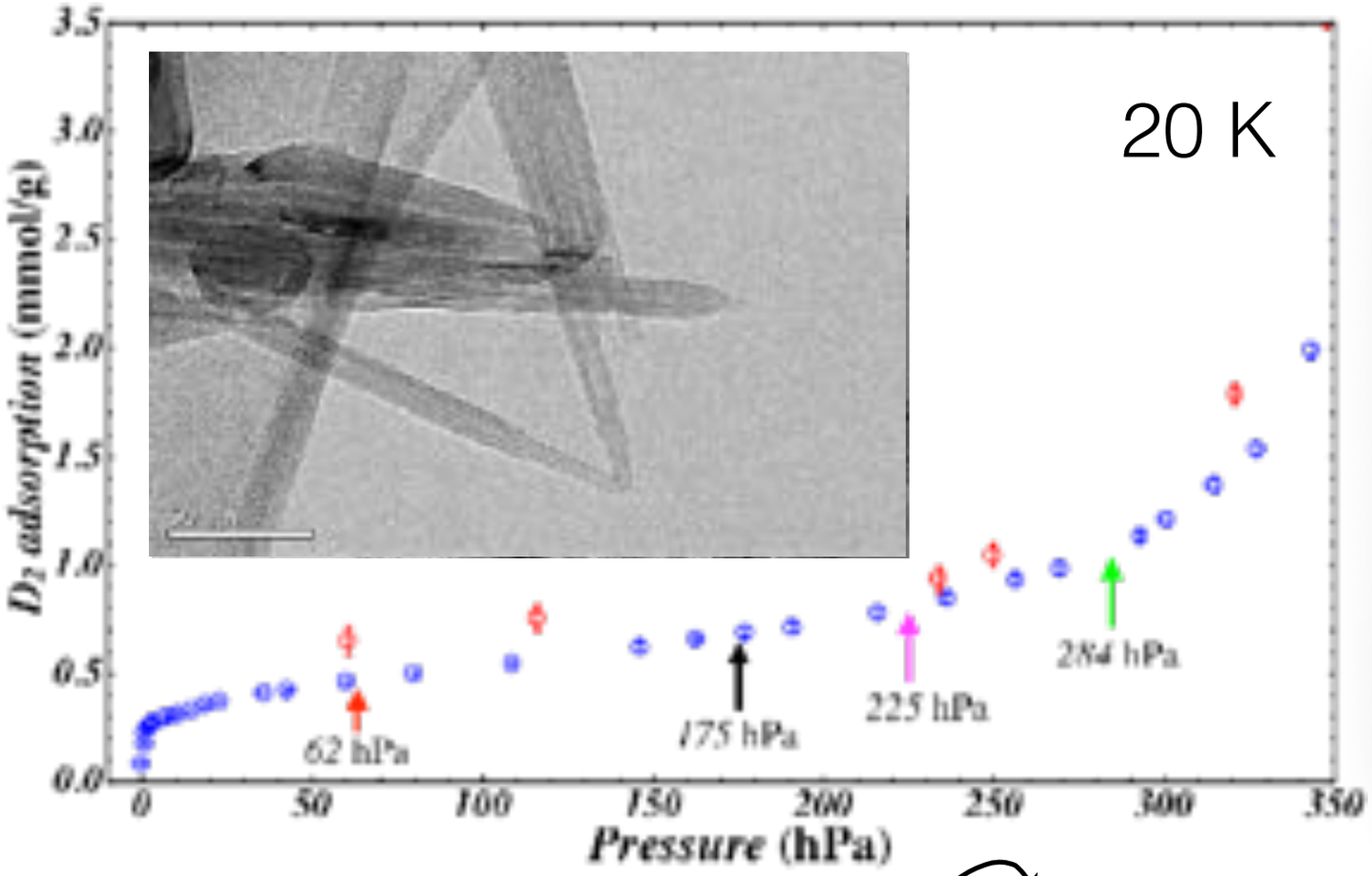


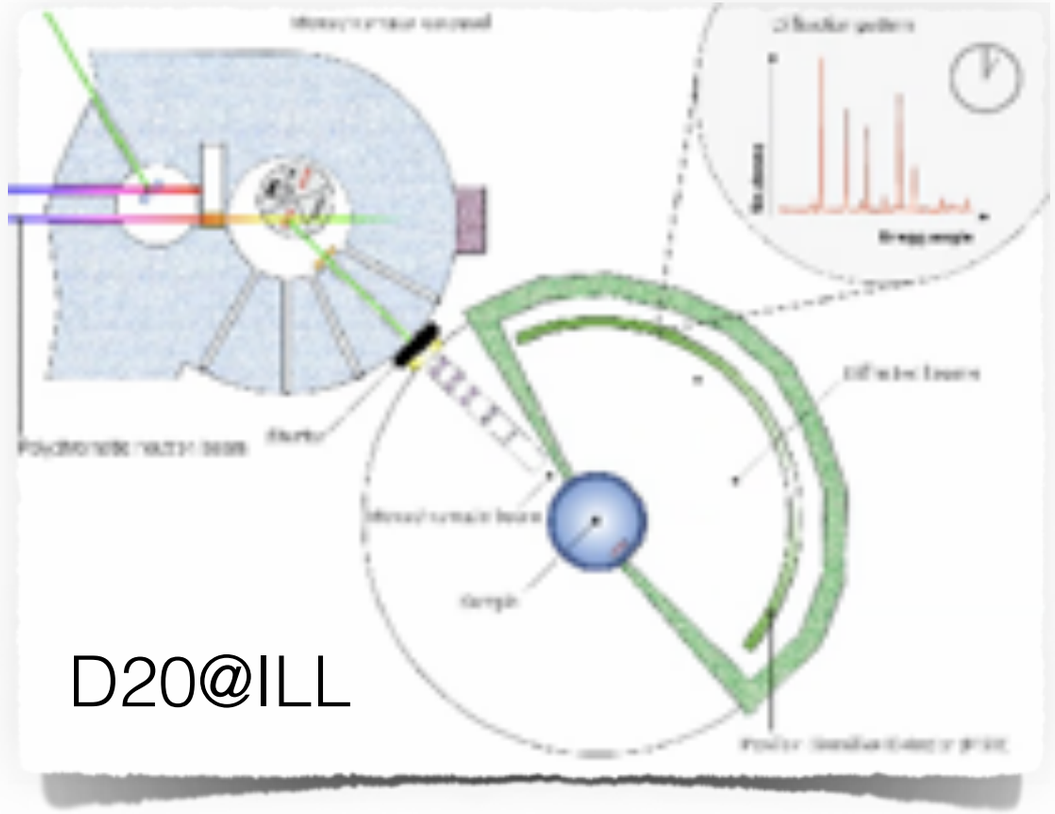


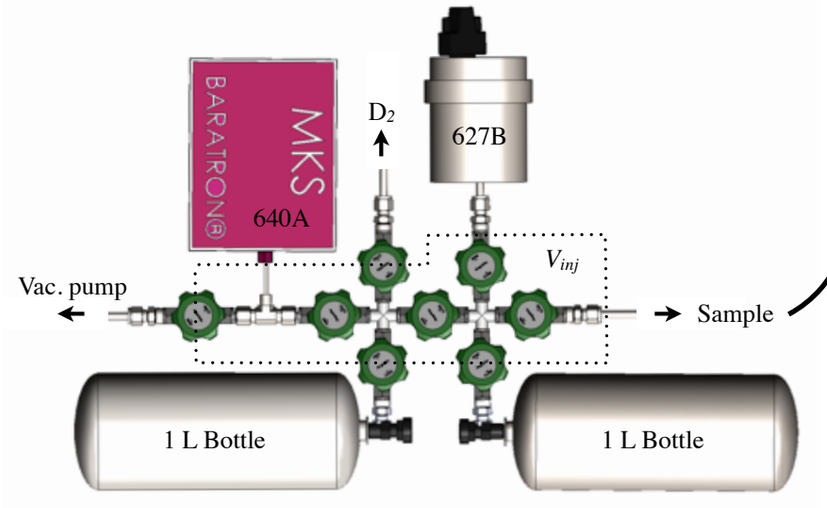
Protocol

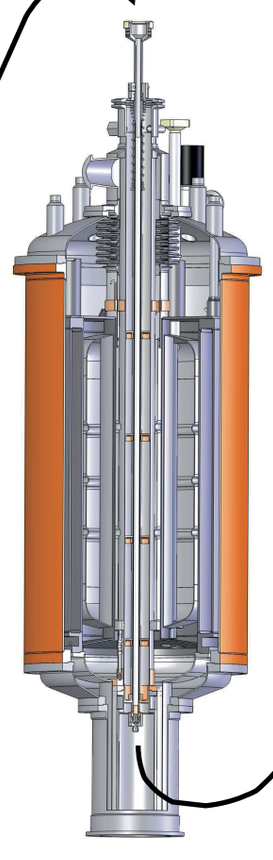
- D_2 instead of H_2
- First load at 20 K until a barely discernible signal appears
- Heat up to 24.5 K
- Slow cooling/heating cycle (0.1 K each 70 s) down to 2 K
- Repeat increasing load at 20 K

1D Crystallisation: our experiment









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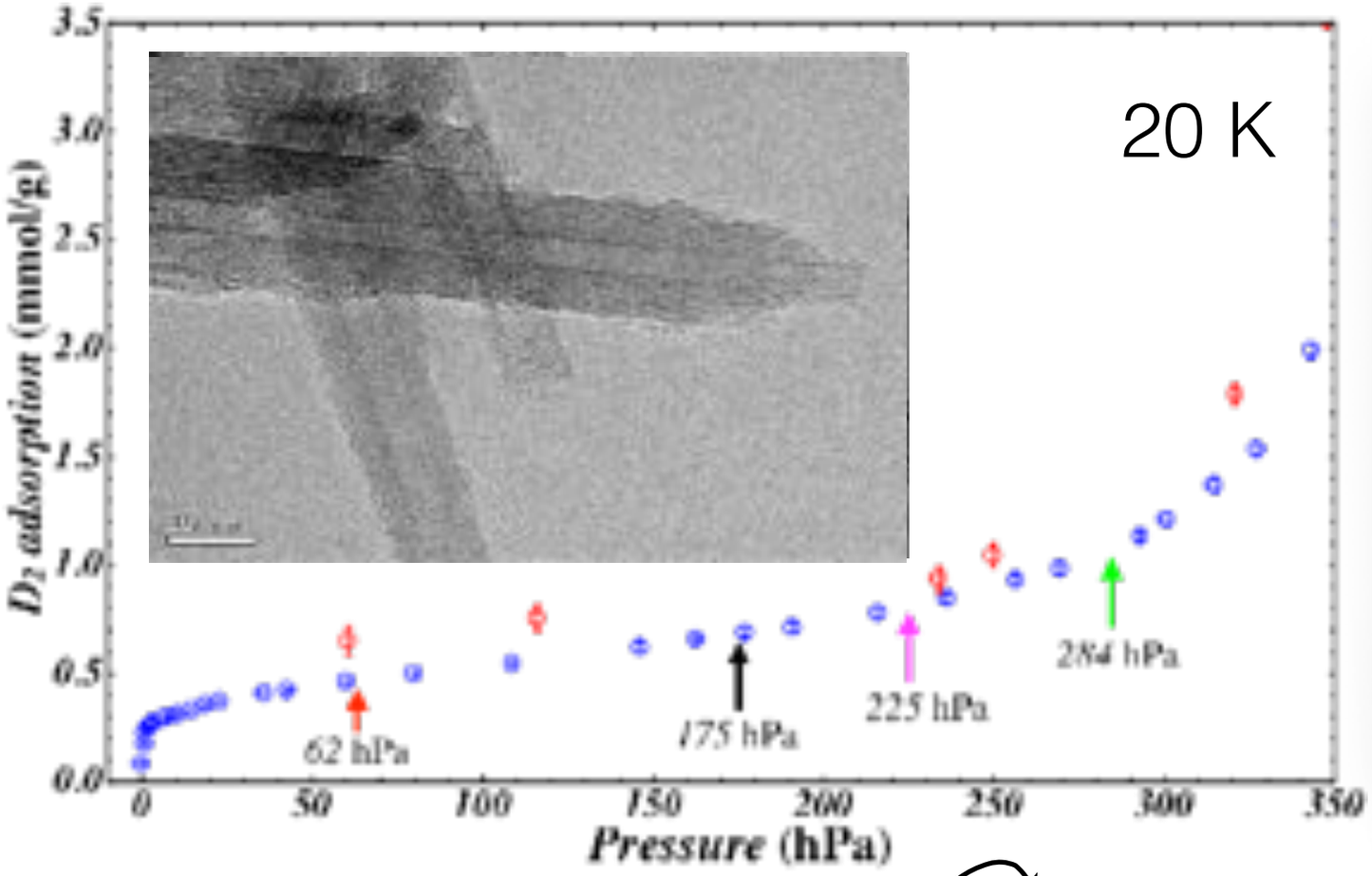

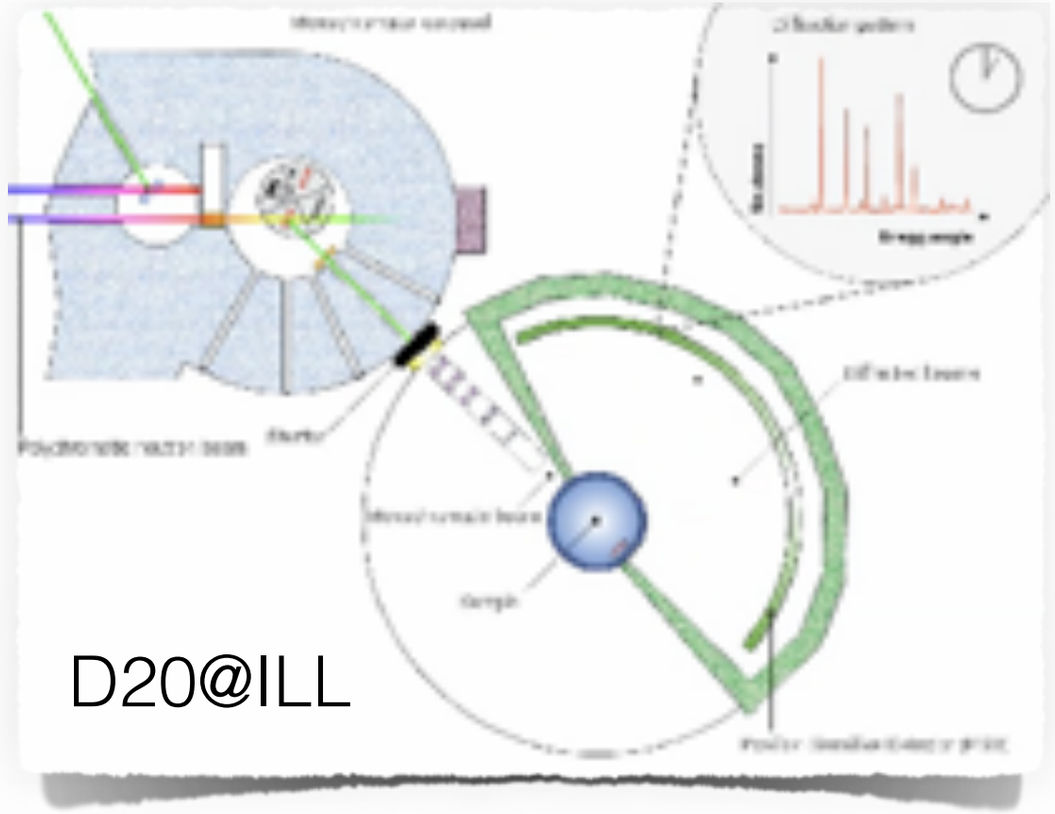

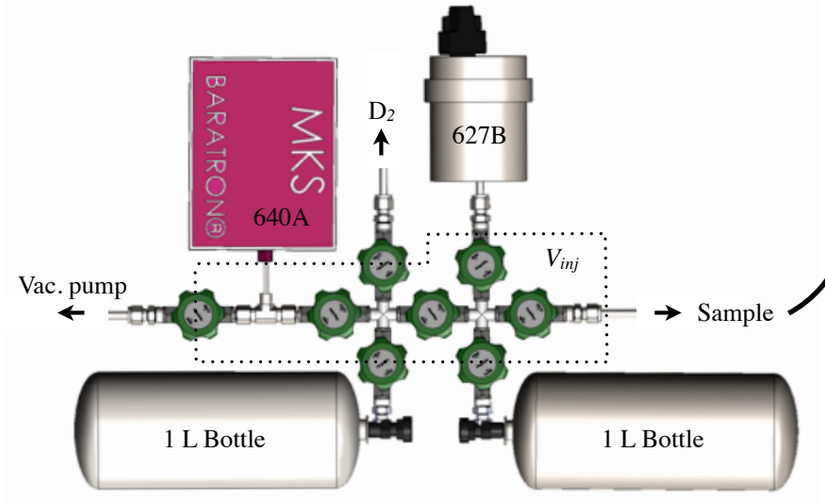

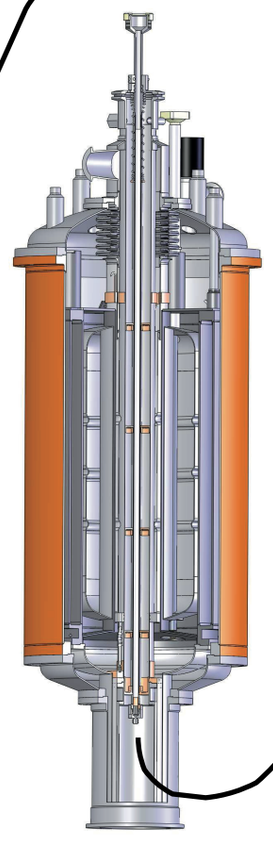

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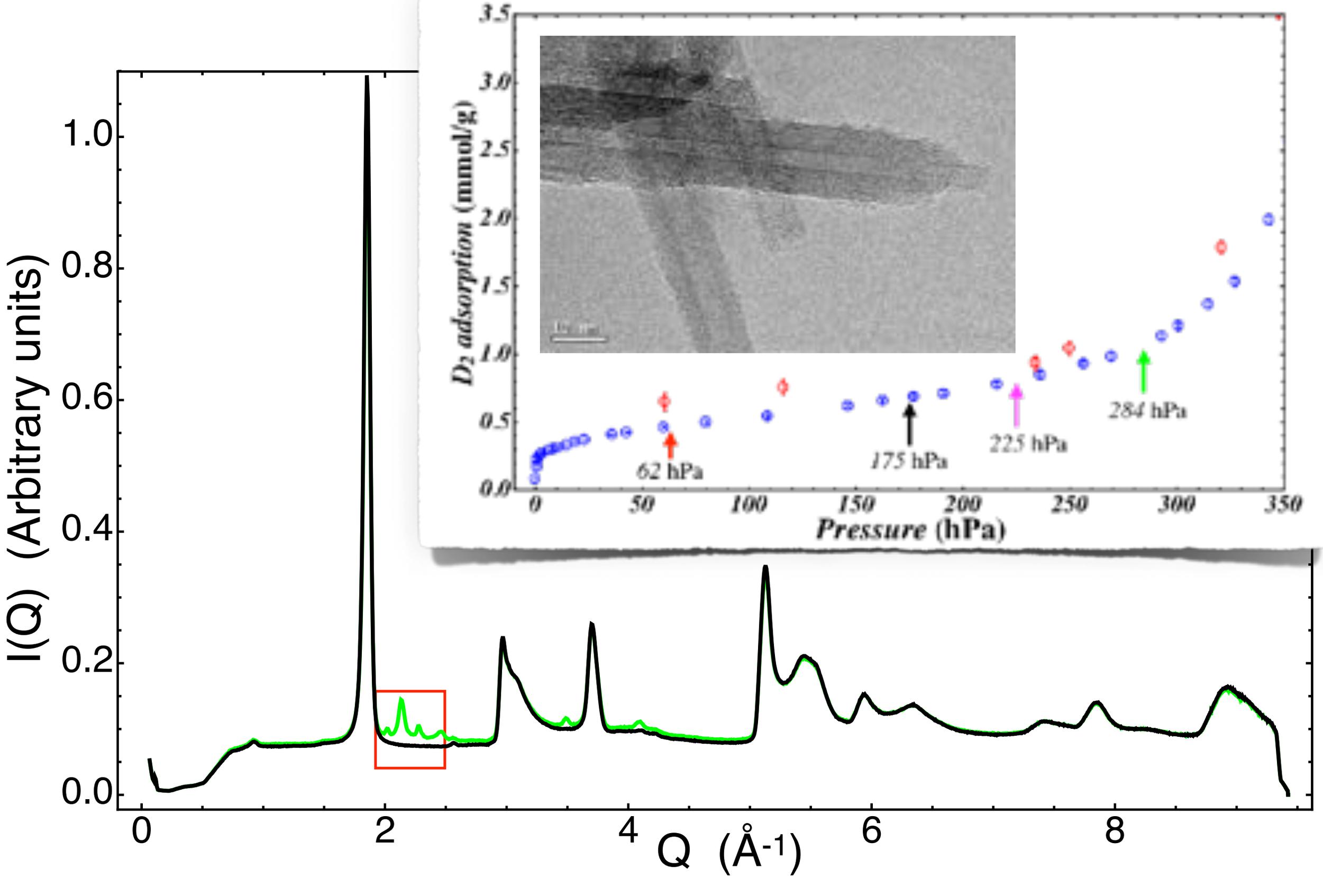
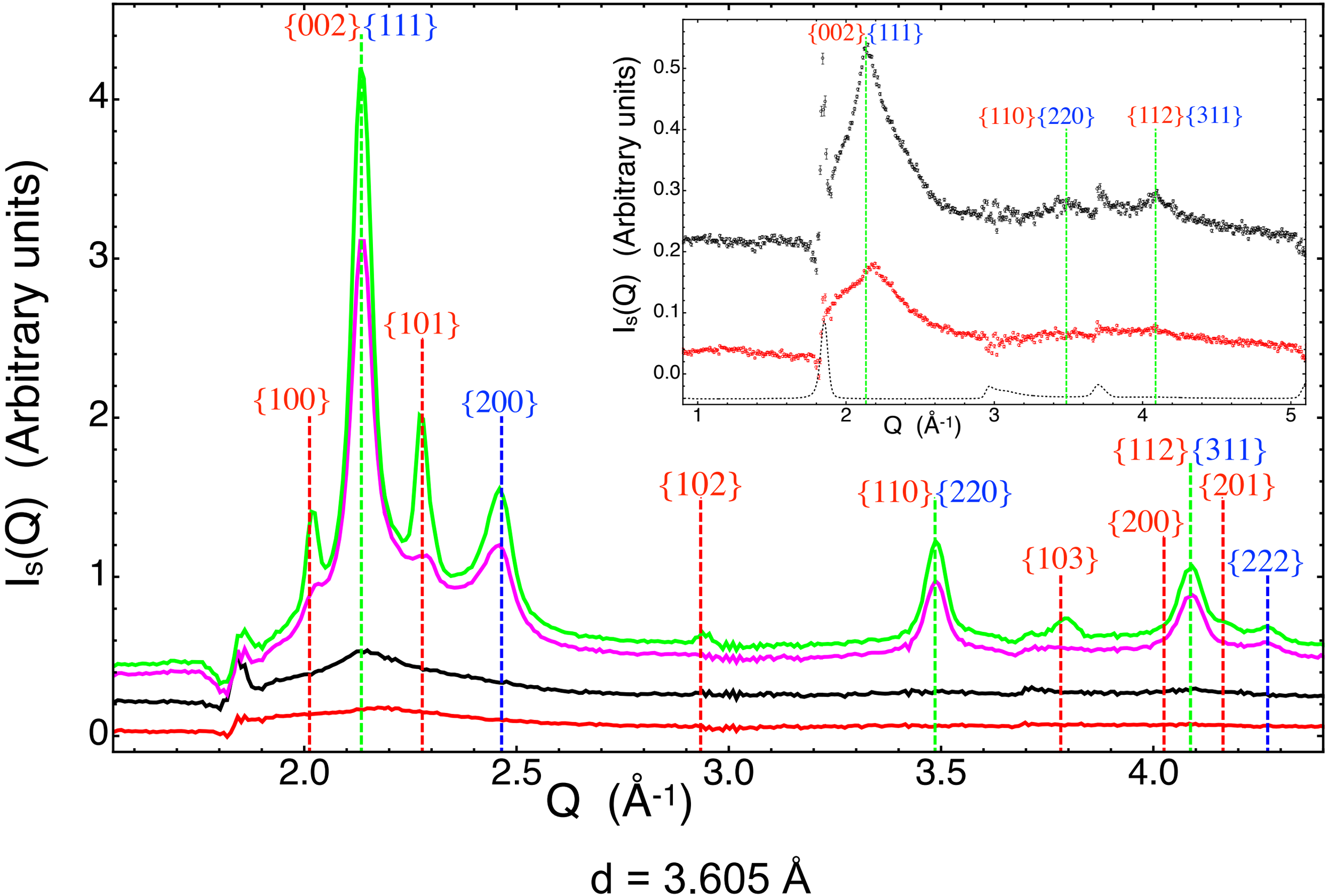
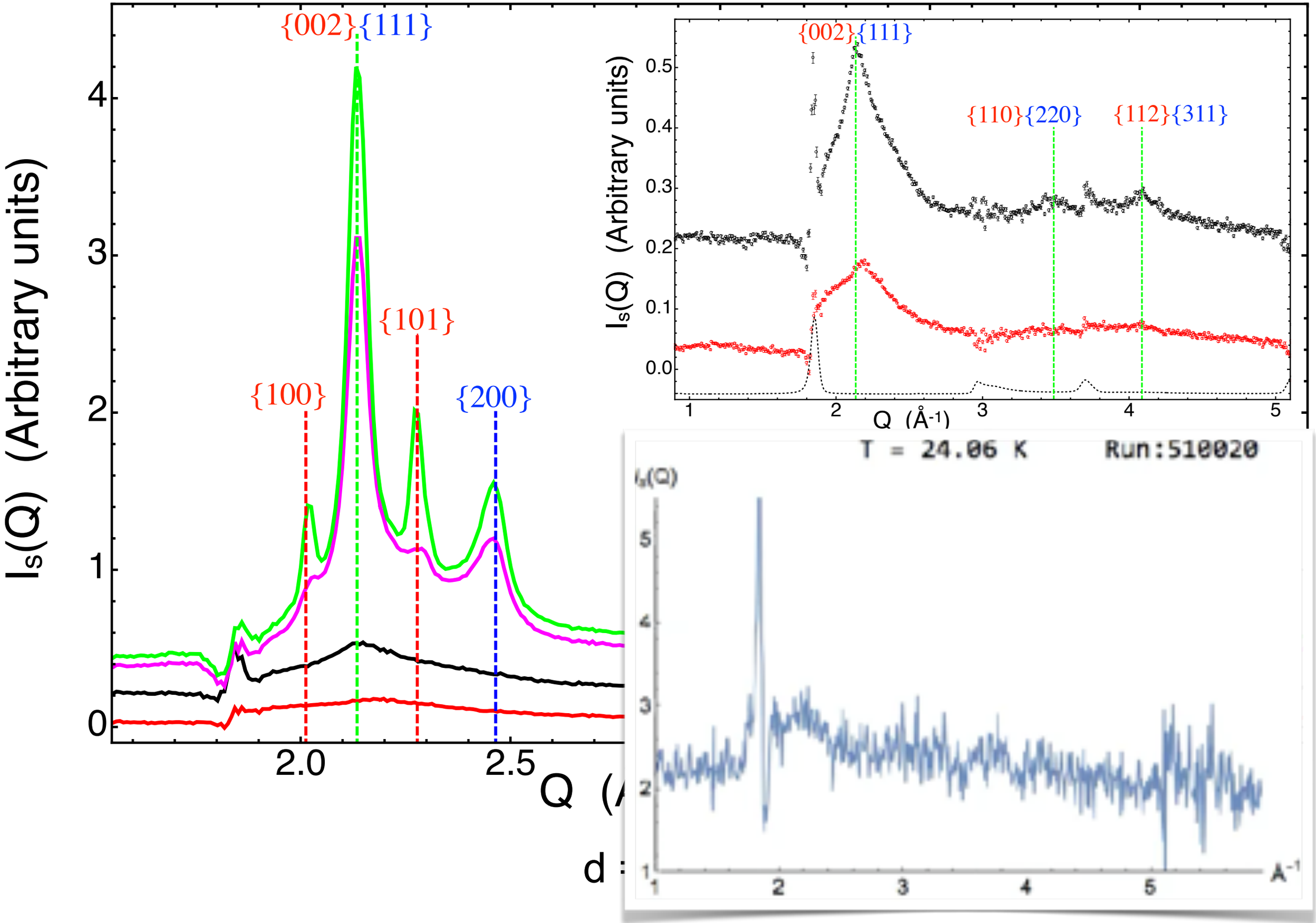

I(Q) (Arbitrary units)
Q (Å-1)
0.0
0.2
0.4
0.6
0.8
1.0
0
2
4
6
8
D2 adsorption (mmol/g)
Pressure (hPa)
0.0
0.5
1.0
1.5
2.0
2.5
3.0
3.5
0
50
100
150
200
250
300
350
62 hPa
175 hPa
225 hPa
284 hPa


{002}{111}
{101}
{100}
{200}
{102}
{110}{220}
{103}
{112}{311}
{201}
{222}
Is(Q) (Arbitrary units)
Q (Å-1)
d = 3.605 Å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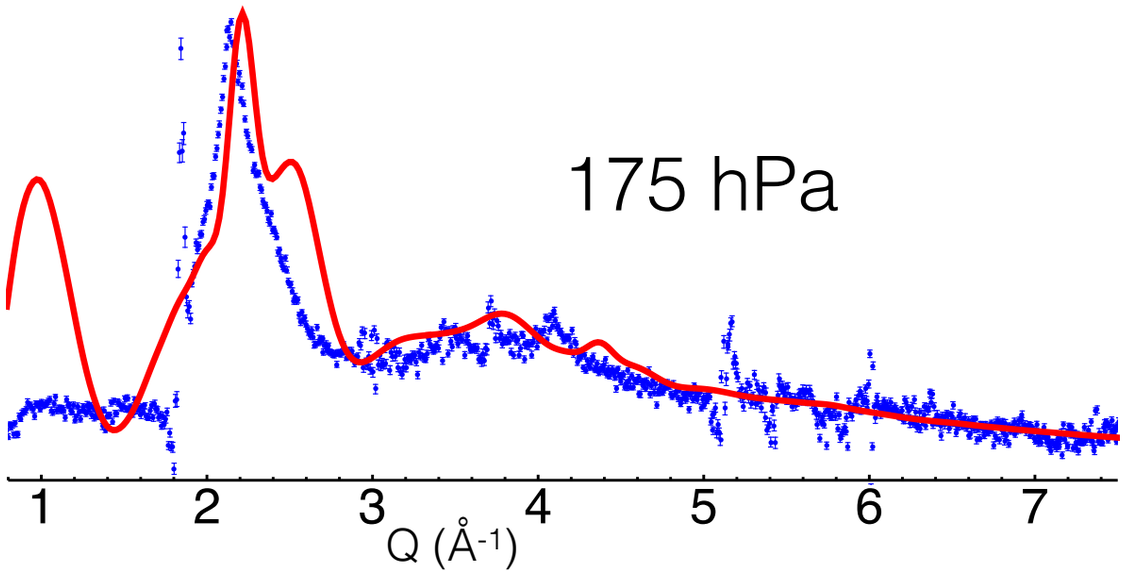
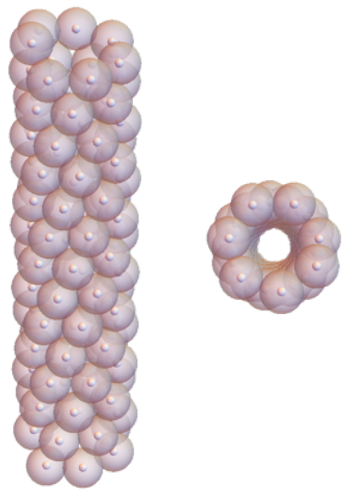
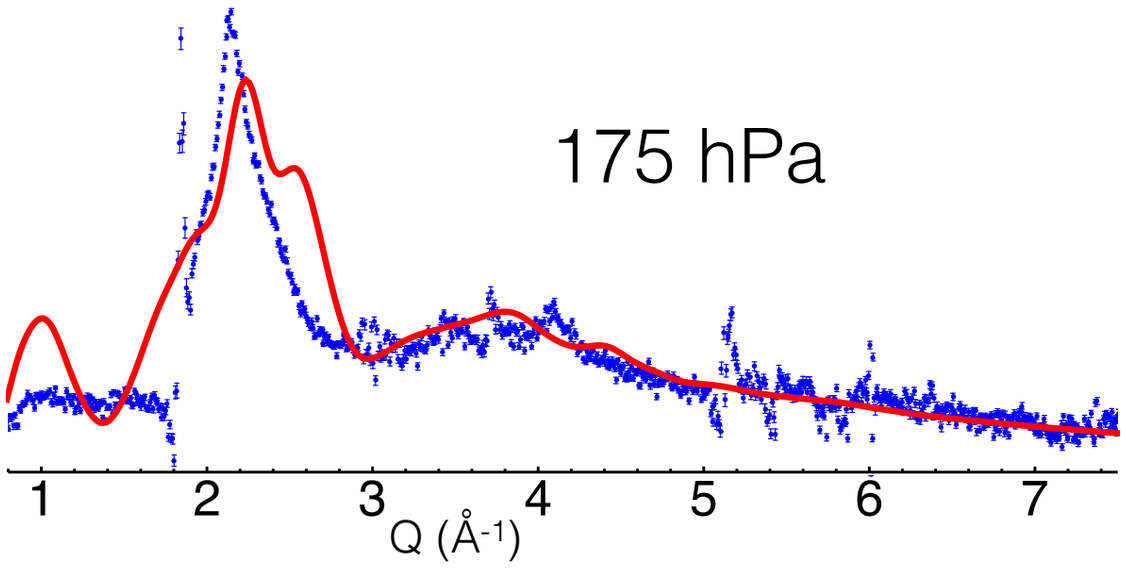
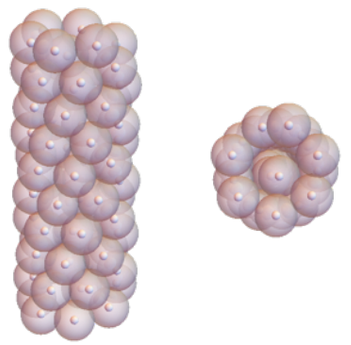
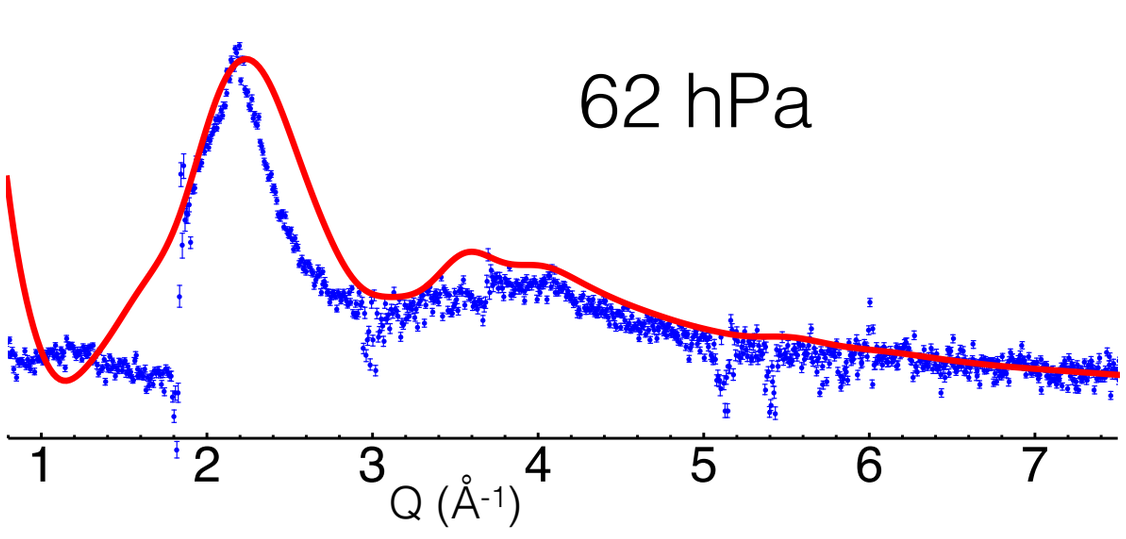
{100}
{200}
{110}{220}
{112}{311}
$I_s(Q)$ (Arbitrary units)
Q (Å^{-1})
T = 24.06 K
Run:510020
d :

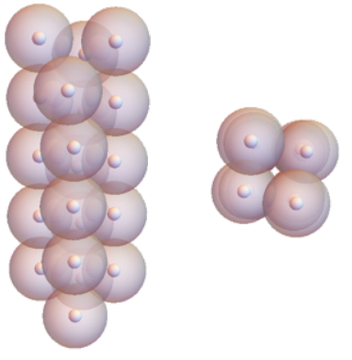

175 hPa
1
2
3
4
5
6
7
Q (Å-1)




175 hPa
1
2
3
4
5
6
7
Q (Å-1)



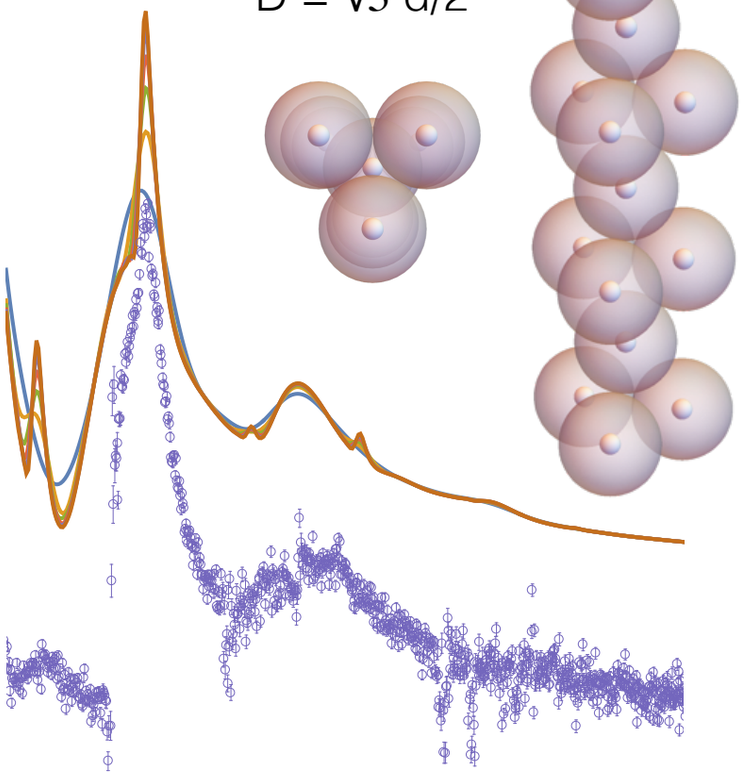

62 hPa
1
2
3
4
5
6
7
Q (Å-1)



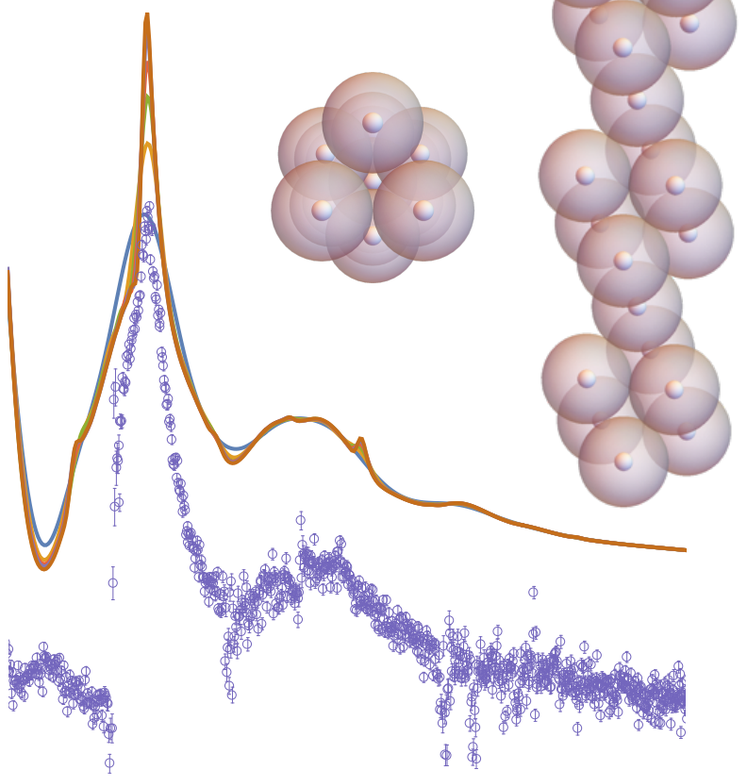
62 hPa

HCP

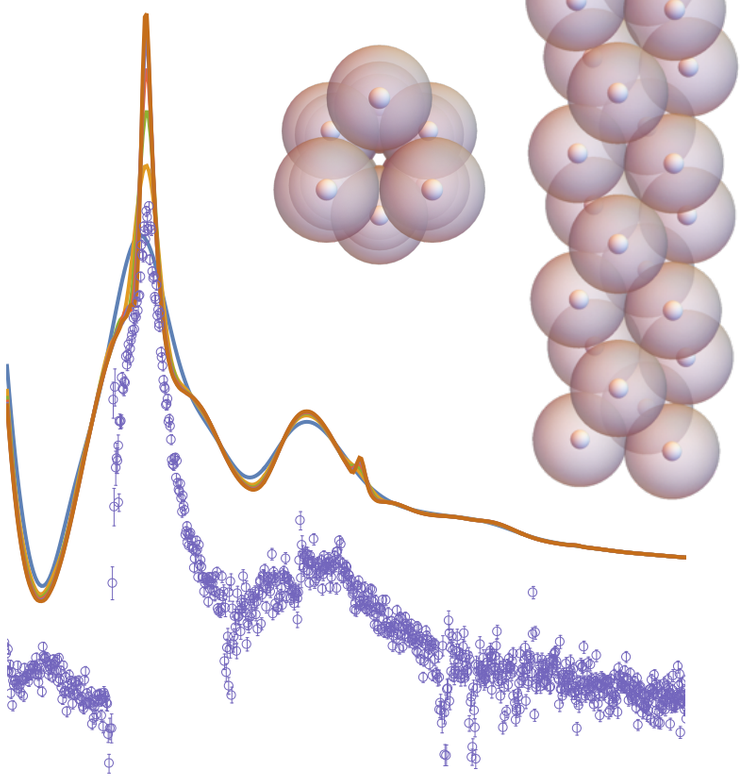
D = √3 d/2



FCC

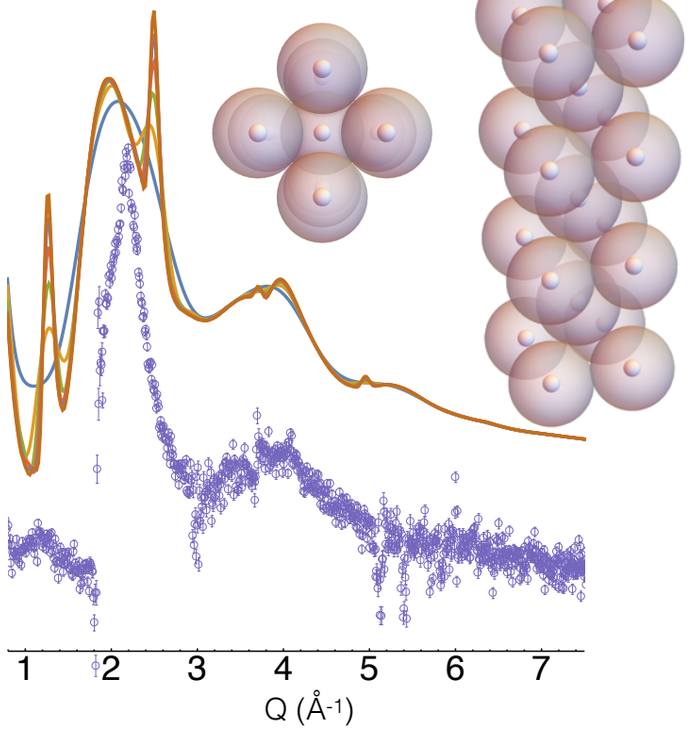


HCP



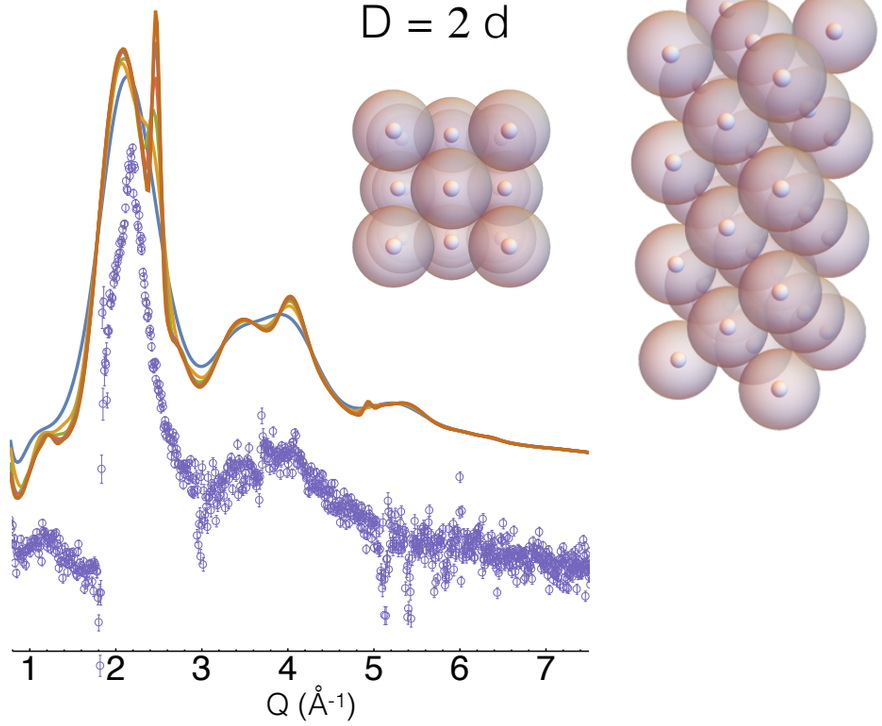
FCC

D = √2 d

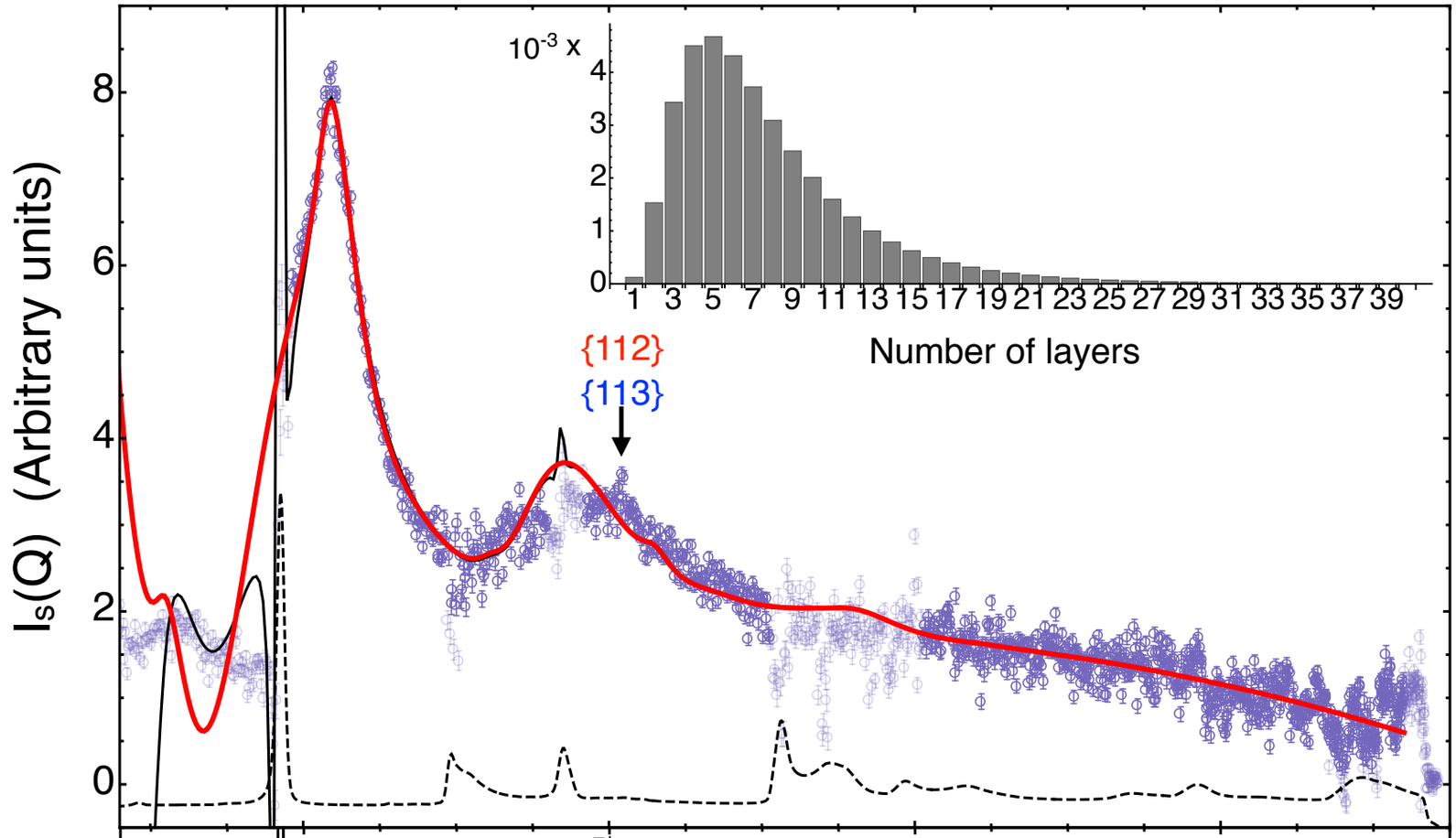


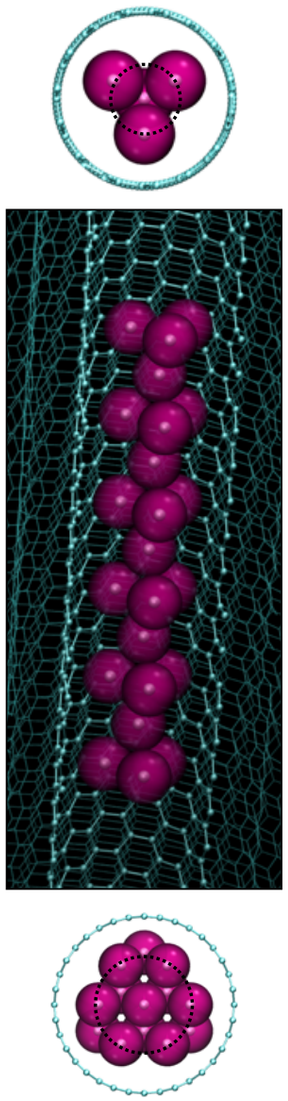
FCC

D = 2 d

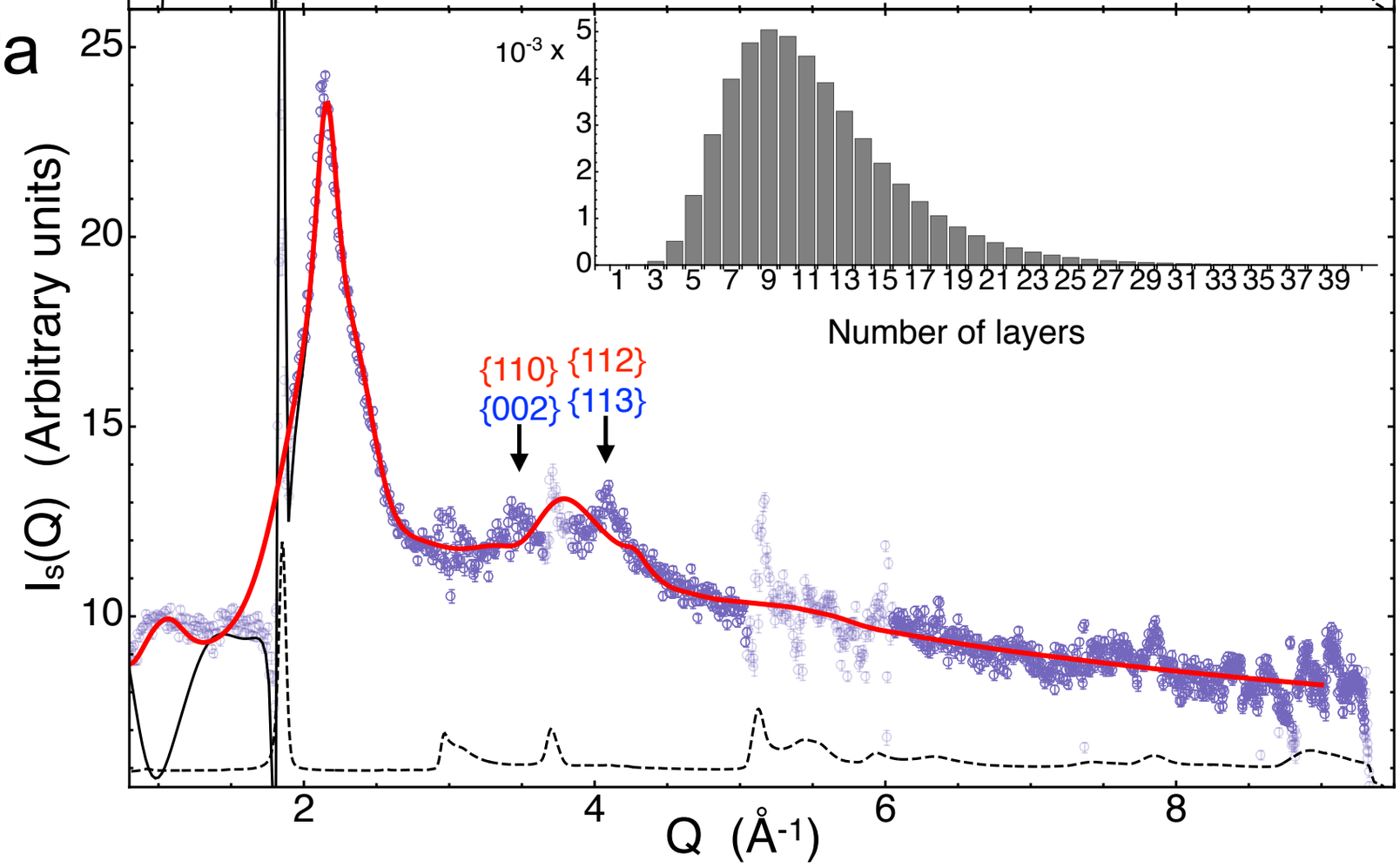


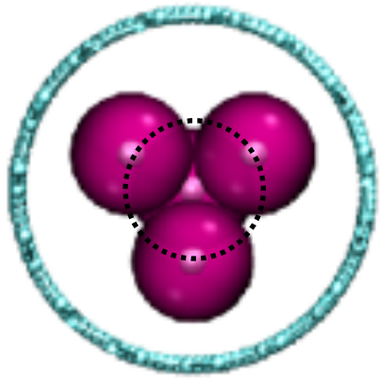
62 hPa

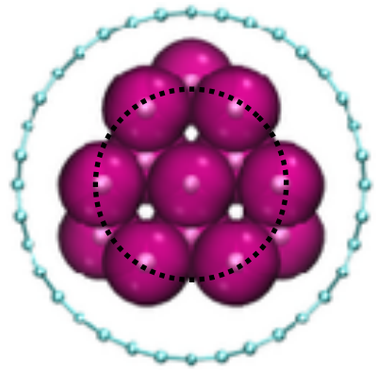


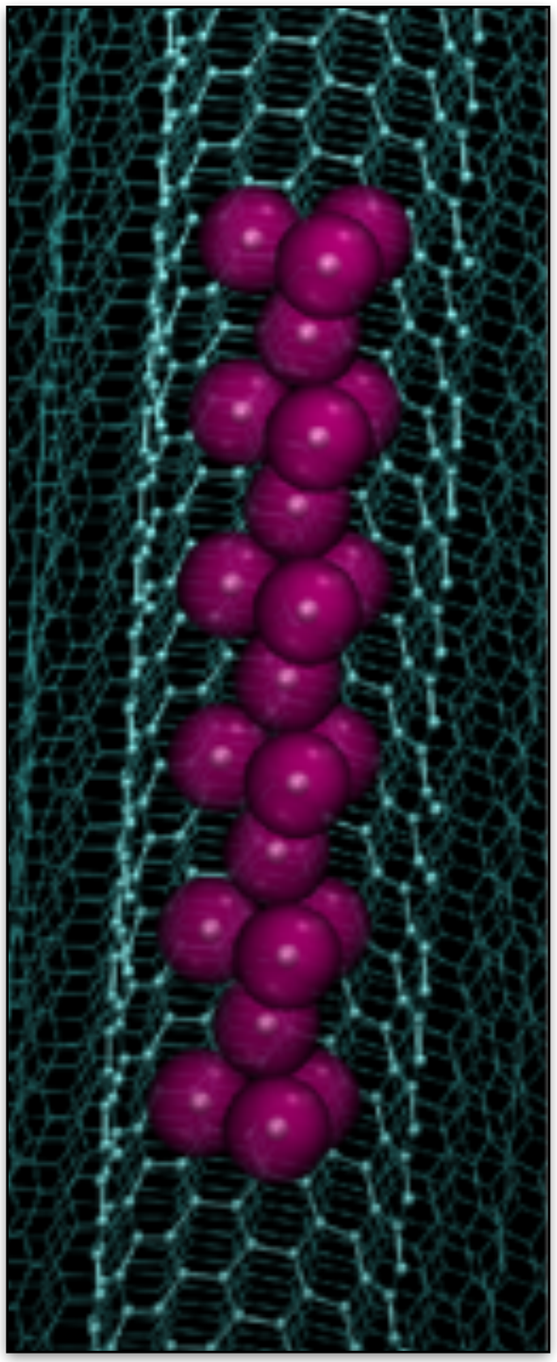


175 hPa

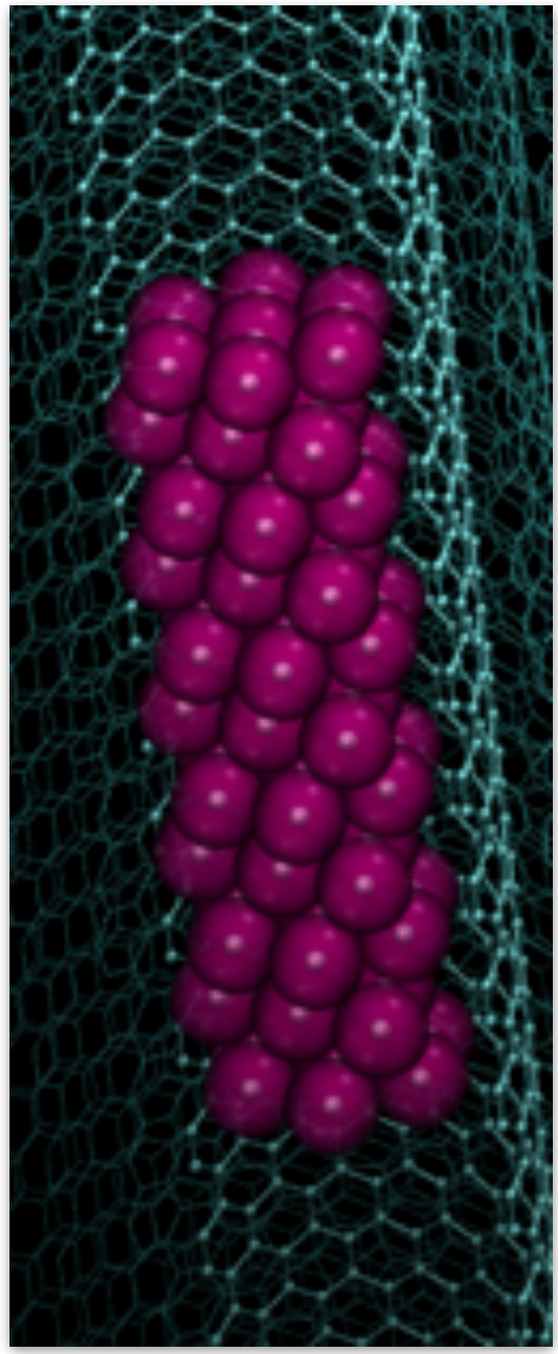








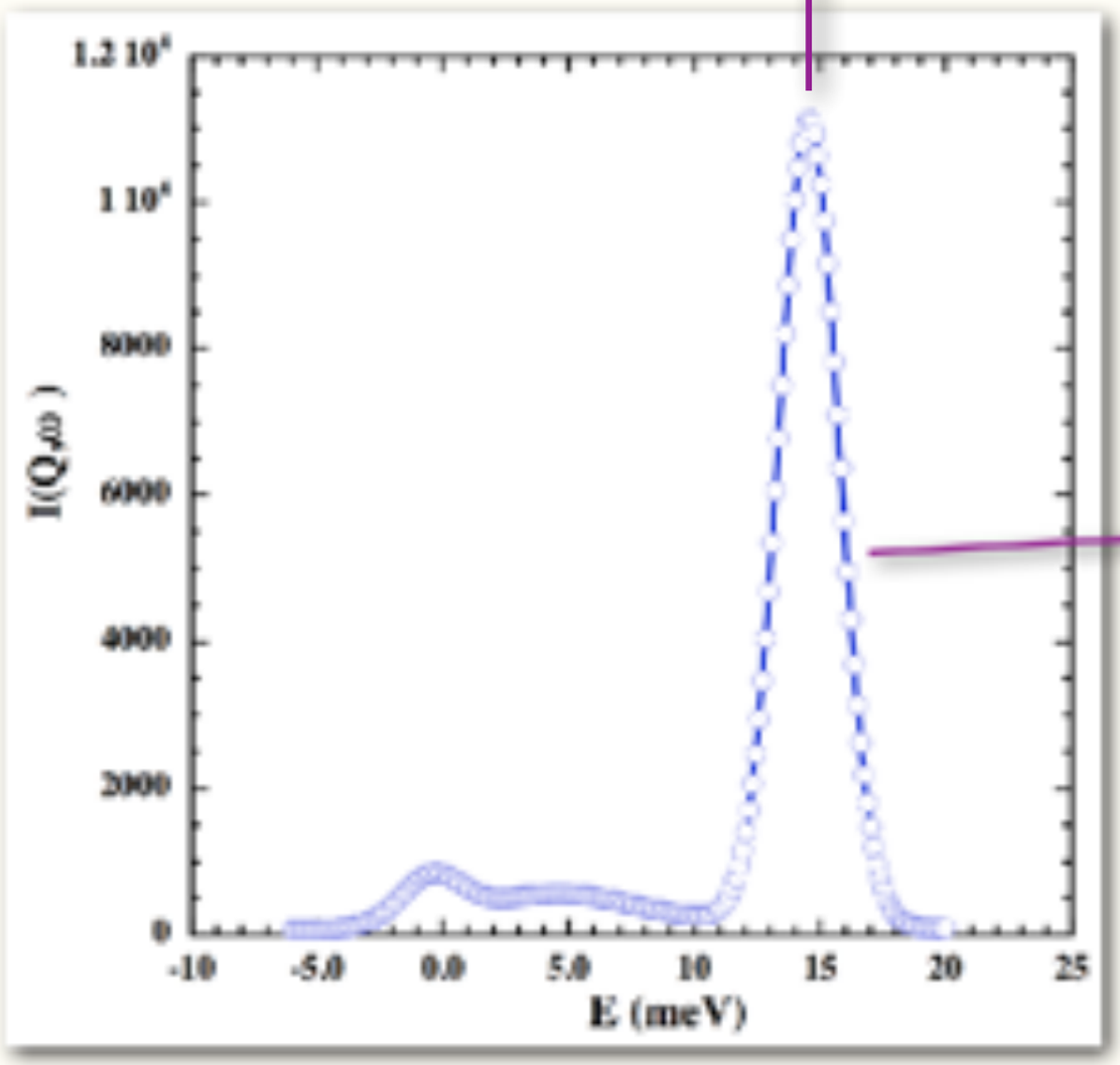
Quantum nuclear effects must be essential to stabilise the 1D Crystals

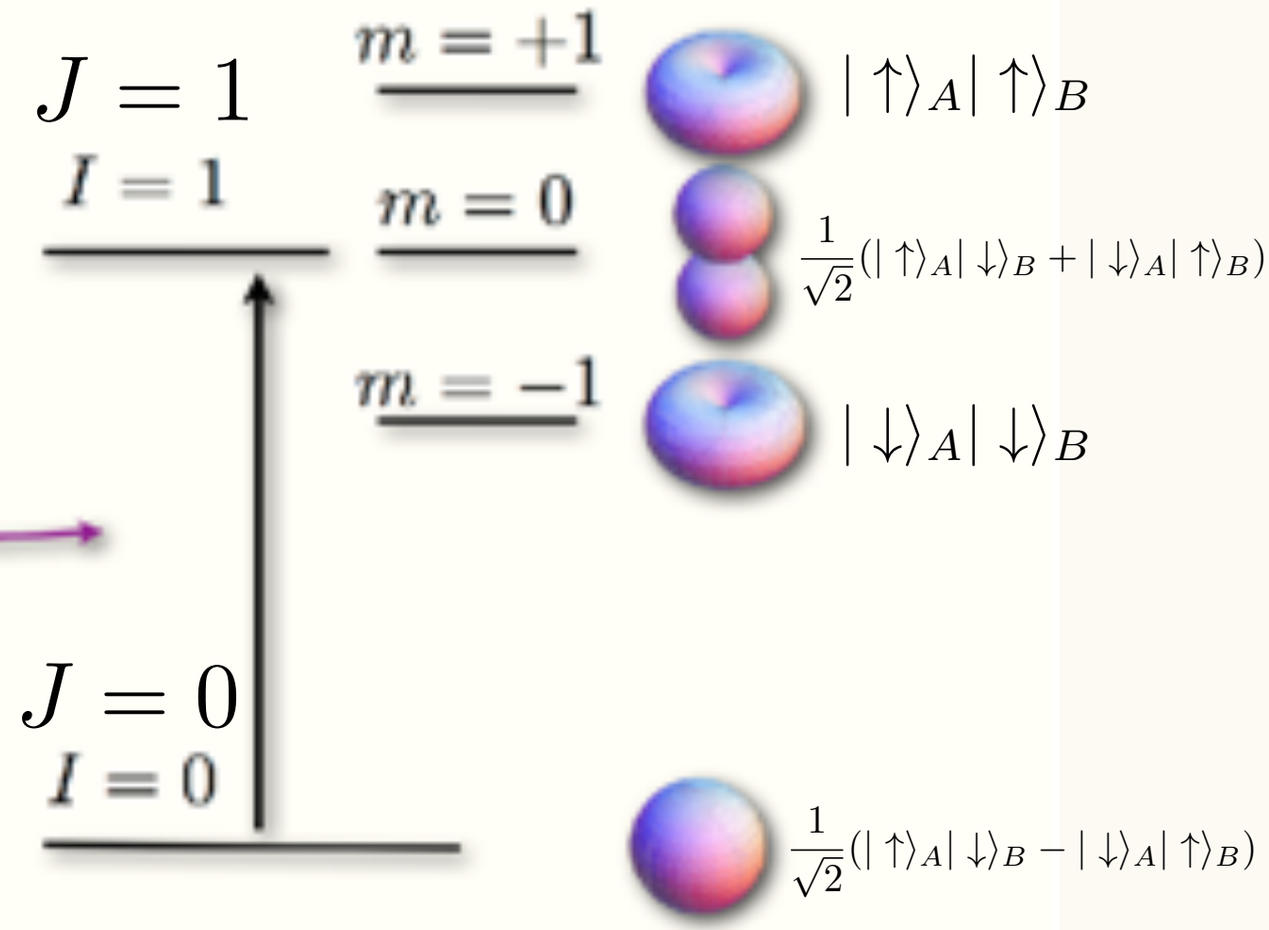


H_2 quantum aspects

Rotational degrees of freedom

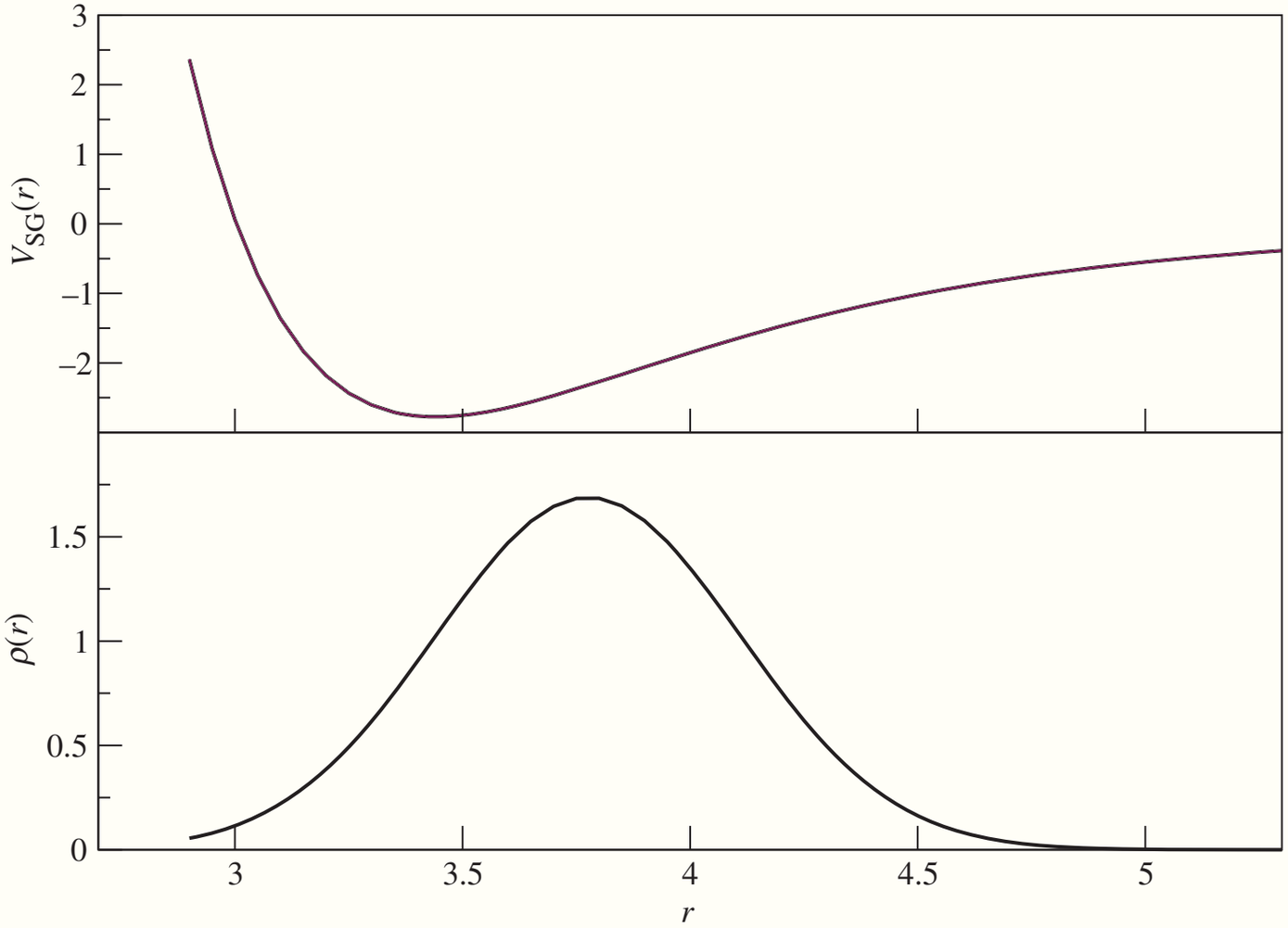
$$E_{01} \simeq 14.6 \text{ meV} \rightarrow \ T \simeq 169 \text{ K}$$





Molecules in the *J = 0* (fundamental level) are very well approximated by structureless entities
Interaction very well approximated by an isotropic (T independent) potential (Silvera-Goldman)
I. F. Silvera and V. V. Goldman, *J. Chem. Phys.* **69**, 4209 (1978)

Translational degrees of freedom (crystal)



Anharmonic crystal even at low temperatures.
Breakdown of the harmonic approximation around equilibrium position

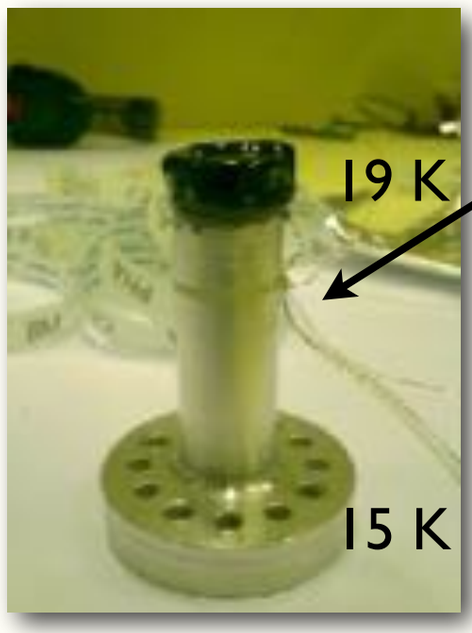
Thermal expansion ~ 0 below a threshold temperature

para-H_2: experimental $T_{tp} = 13.8$ K (*hcp*)

Quasiclassical T_m well above T_{tp} (25 K, ie., ~ 1.8 T_{tp})

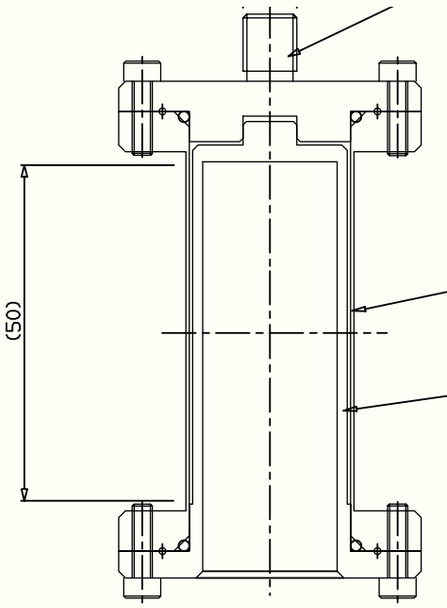
$$\sqrt{\langle u^2 \rangle_{qc}} = 0.75 \text{ Å}$$

Experiment

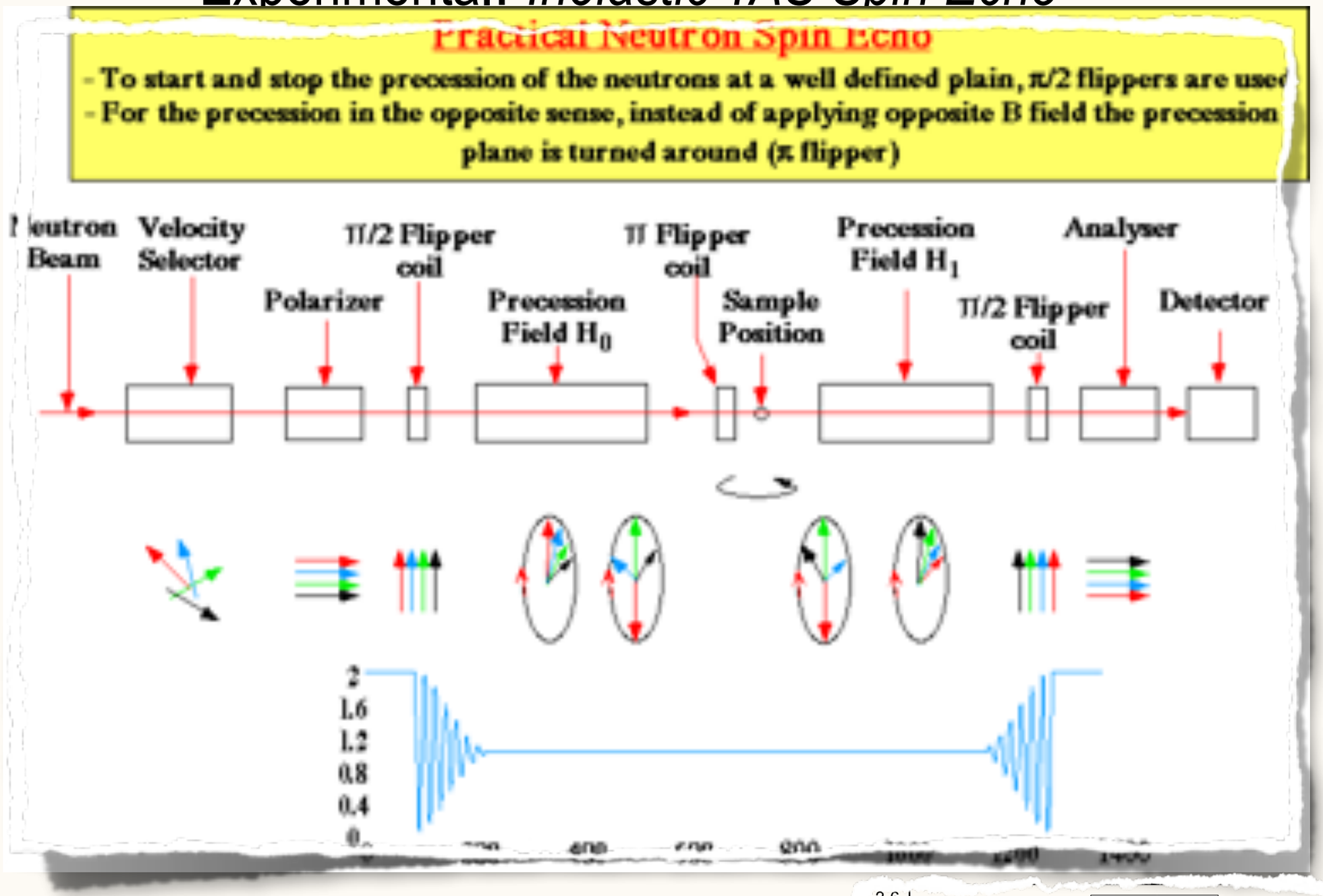


Half filled with
6 g of Oxisorb (CrO_3)

Liquid H_2 were left in
this catalytic cylinder
during 5 days before
loading to the sample can
while cooling to 13 K



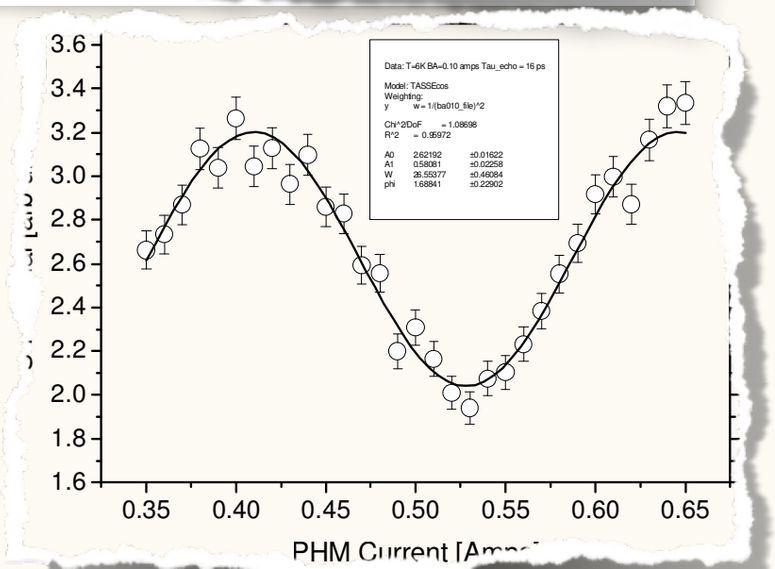
Experimental: *Inelastic TAS Spin Echo*



$$k_f = 2.66 \text{ Å}^{-1}$$

$$(Q, \omega) = (2.5 \text{ Å}^{-1}, 14.7 \text{ meV})$$

Incoherent SE = 1/3 Coherent SE

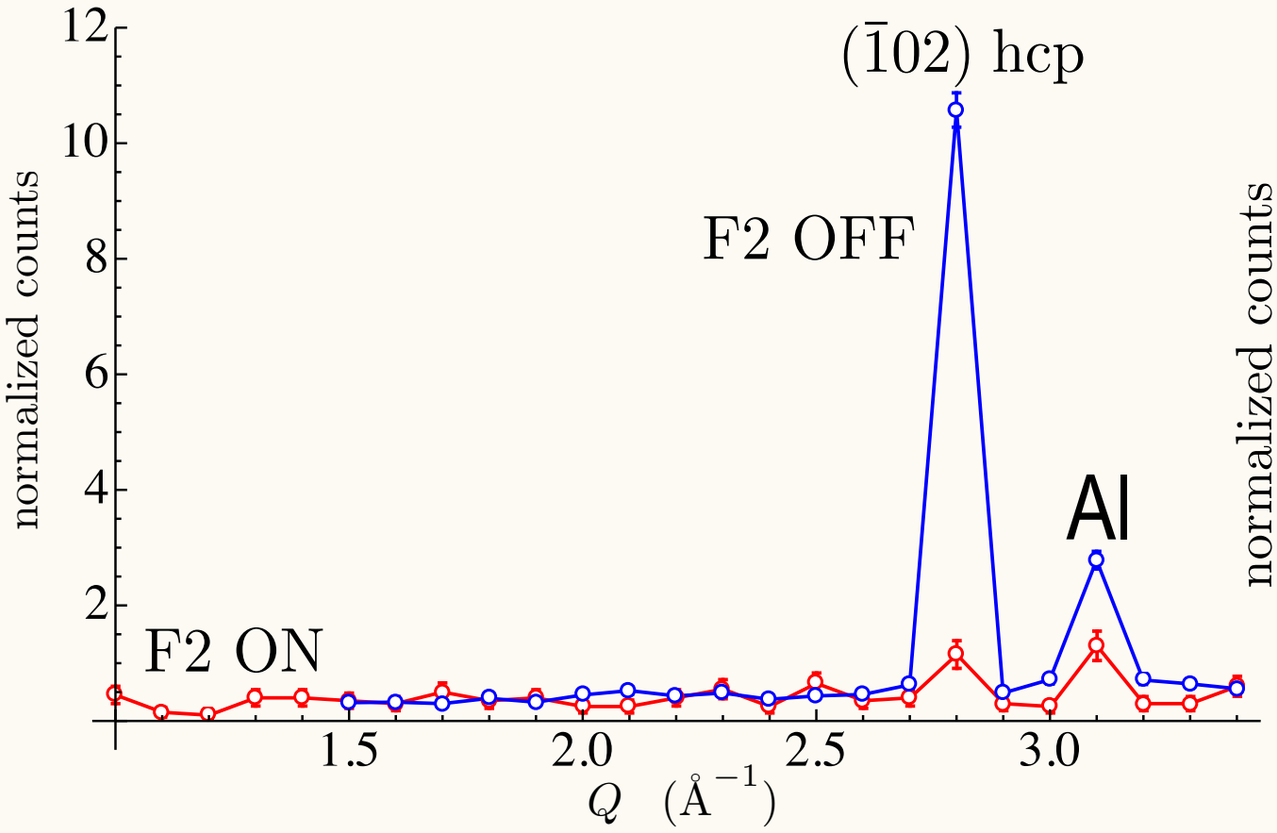


Results

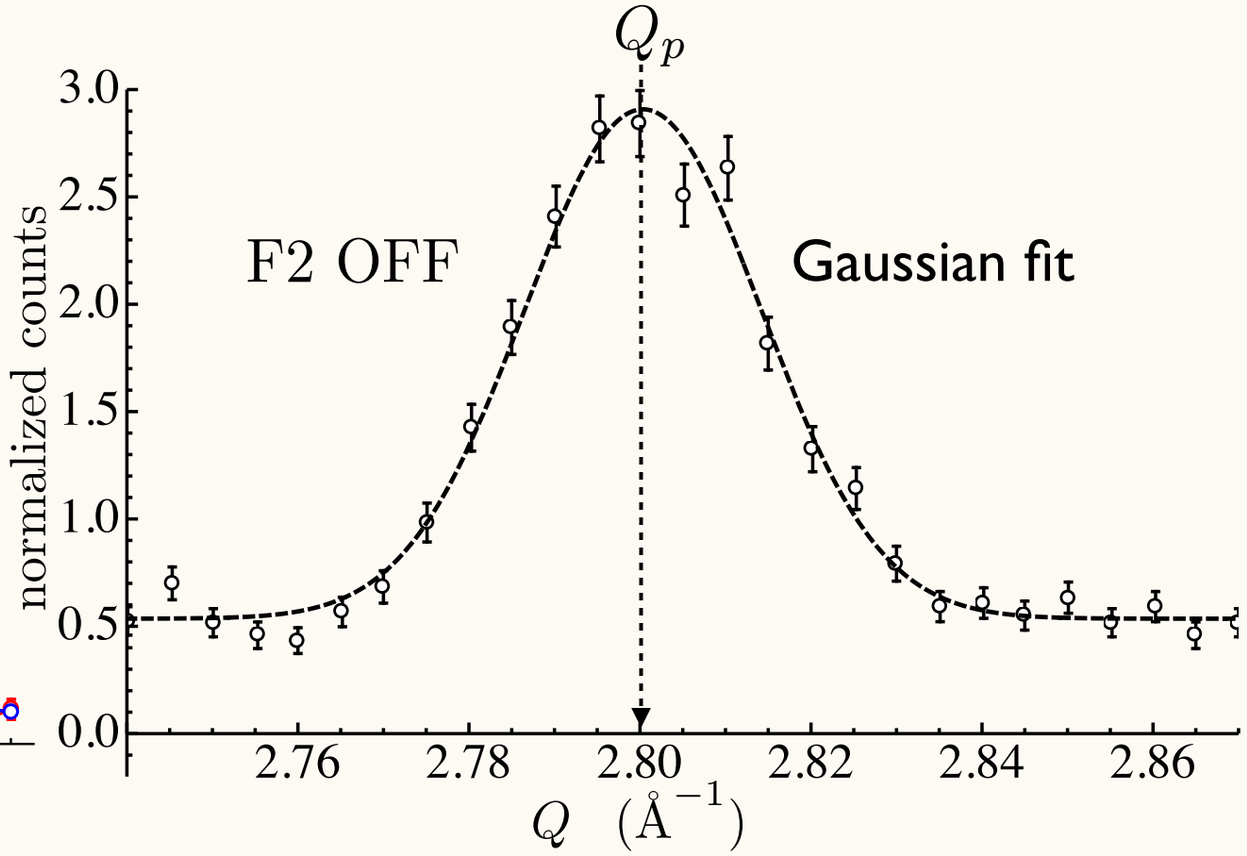
Bragg scattering

F1 OFF, $E = 0$ meV, $T = 13.2$ K

Rough scans



Fine scans around 2.8



- Monocrystalline sample
- High-purity *para*-H_2

$c_0 = 0.001 \pm 0.002$

$Q_p = 2.8004 \pm 0.0008$ Å^{-1}, $T = 13.17$ K, i.e., $0.95\,T_{tp}$

$Q_p = 2.8023 \pm 0.0006$ Å^{-1}, $T = 3.1$ K, i.e., $0.22\,T_{tp}$

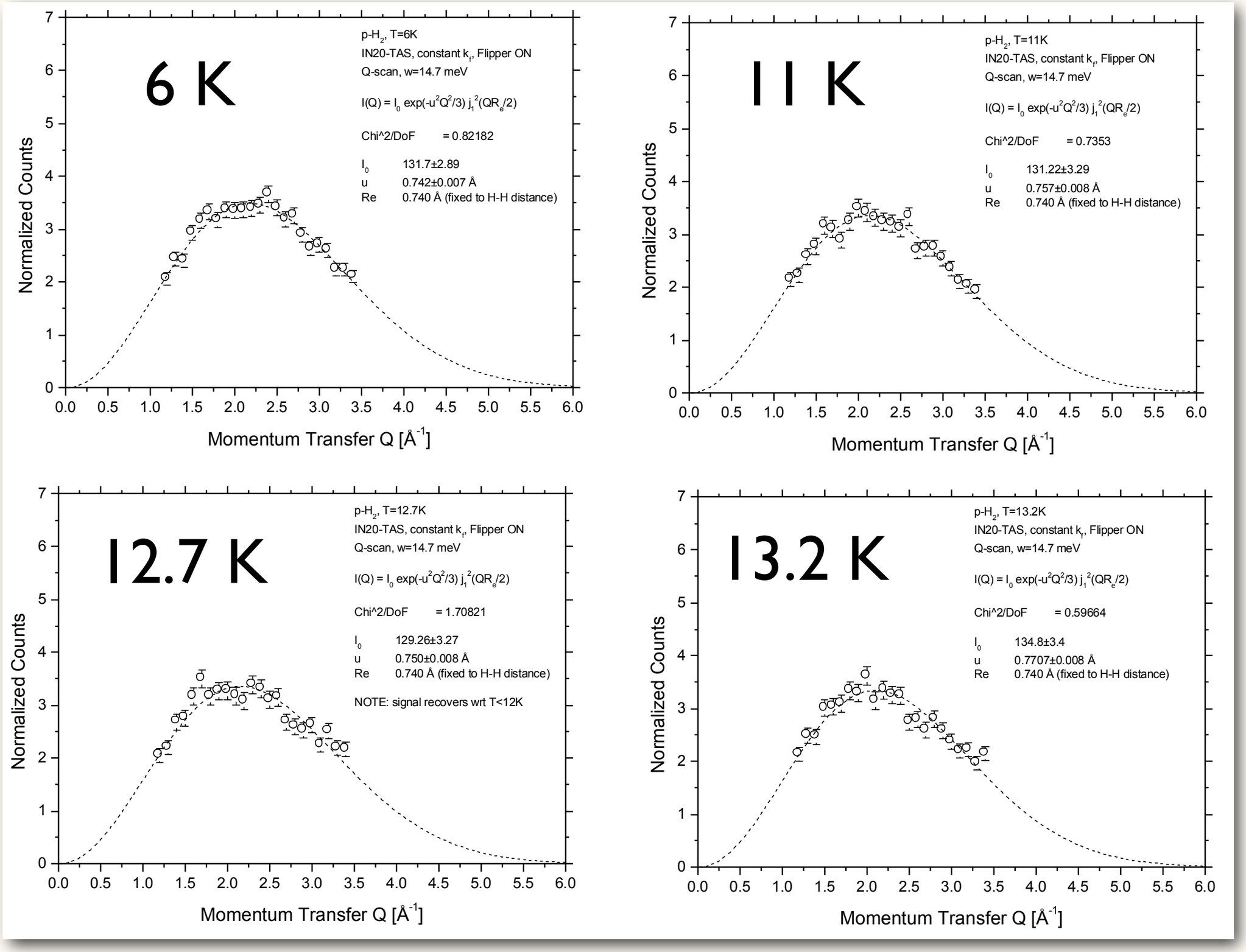
$Q_p(13.7)/Q_p(3.1) = 1.0007$

hcp with $R_{NN} = 3.78$ Å

Results

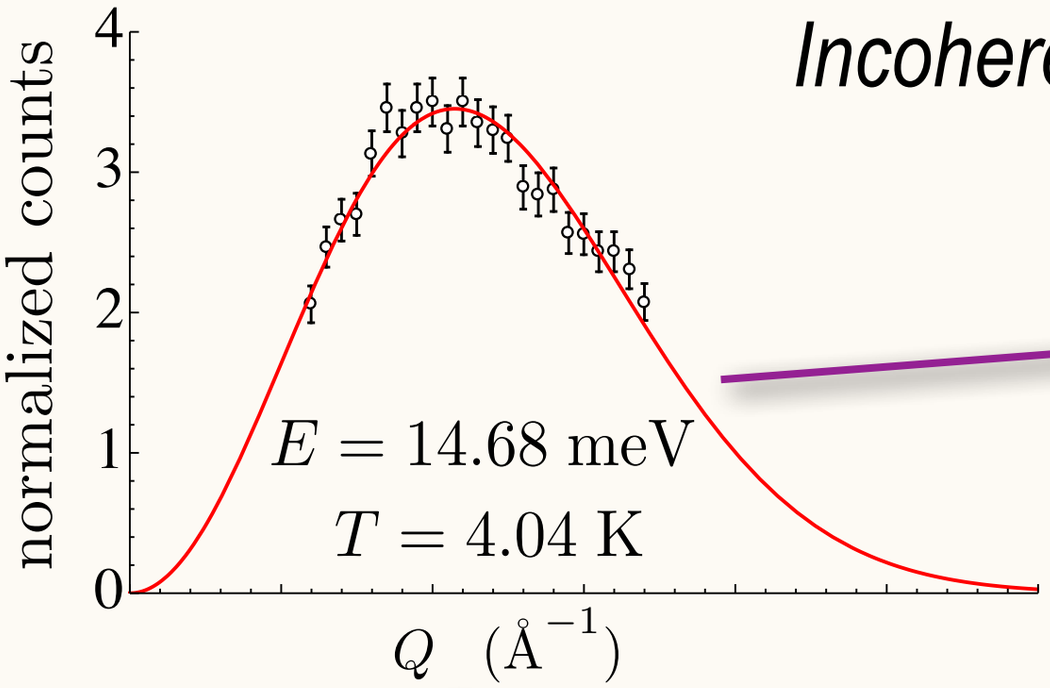
Incoherent Q-scans

F2 ON, $E \simeq 14.7$ meV



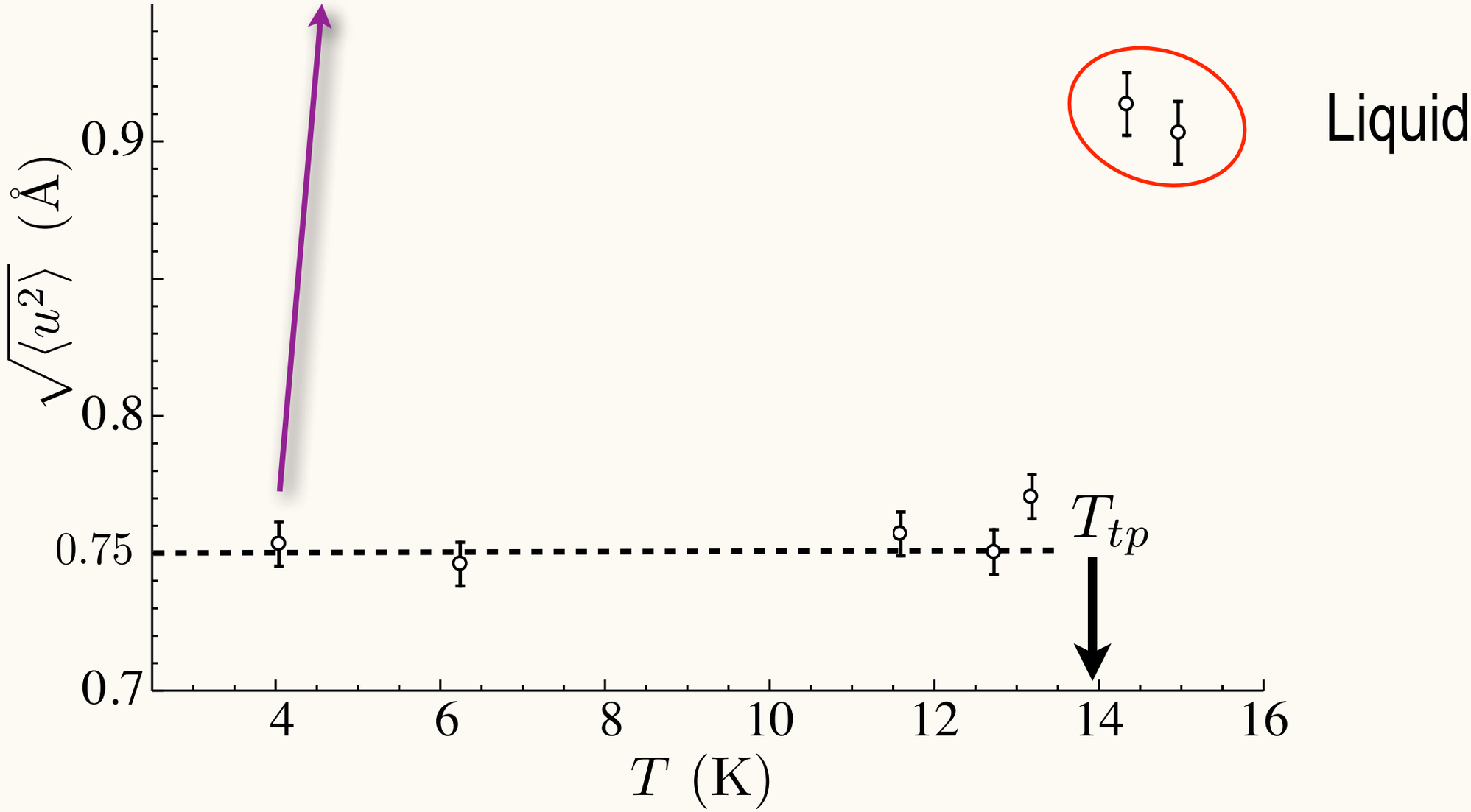
Results

Incoherent Q-scans



$$I(Q) = j_1\left(Q\,d/2\right)\exp\left(-\frac{\langle u^2\rangle}{3}\,Q^2\right)$$

$$d = 0.74\ \text{Å}$$

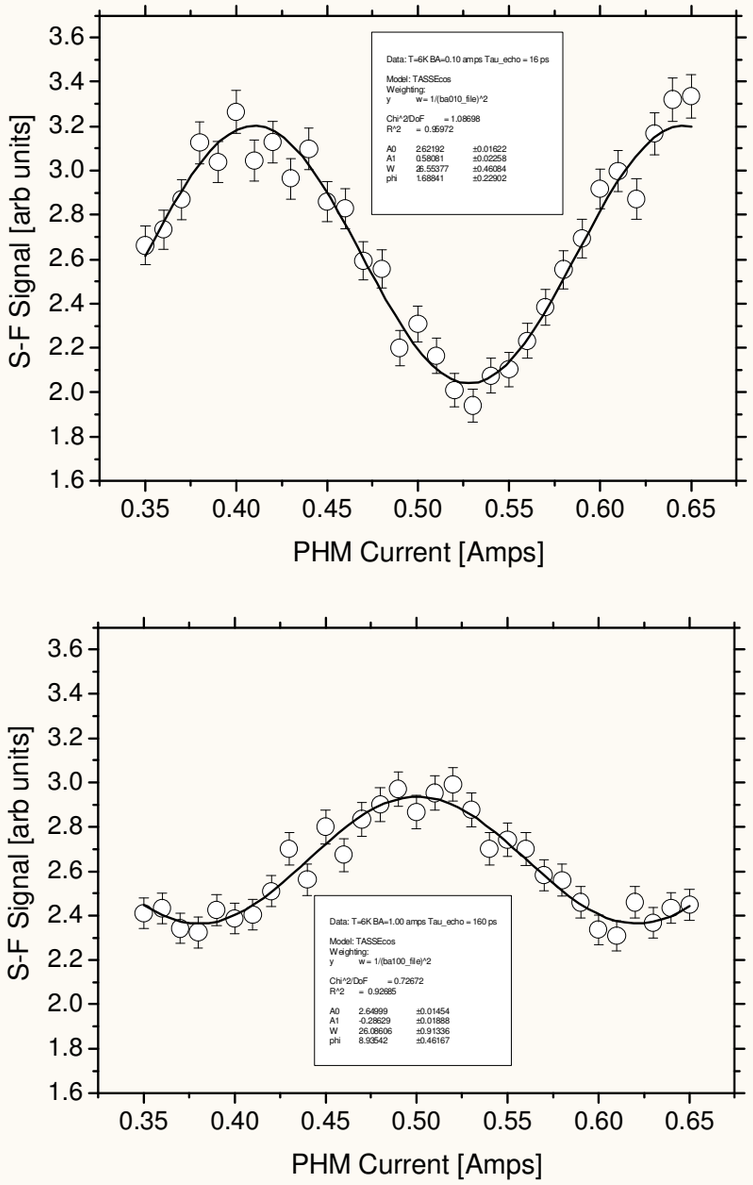


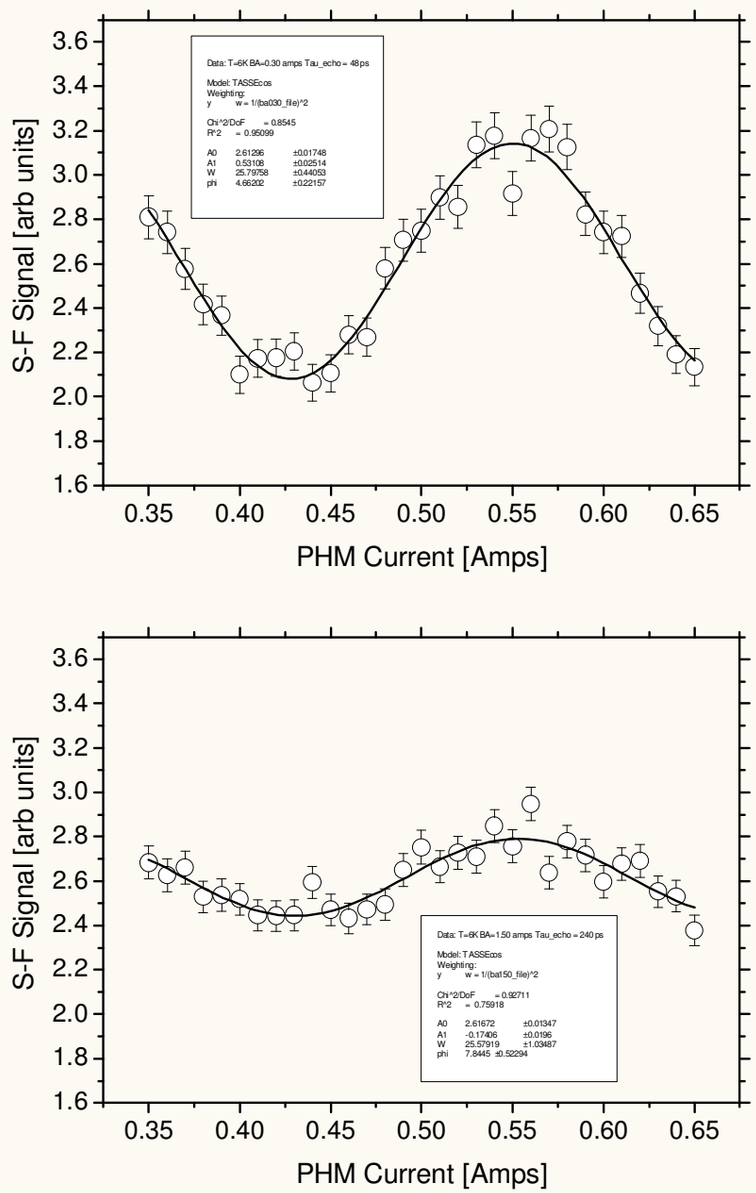
Liquid

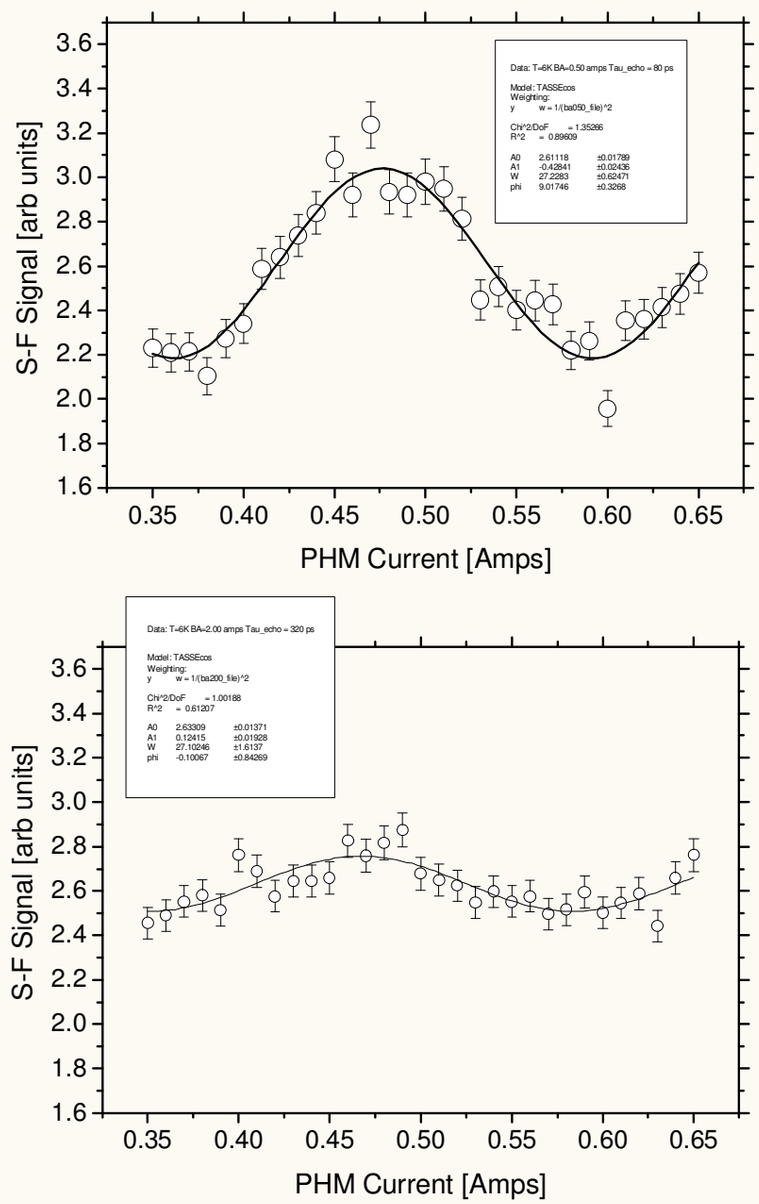
Results

Spin echo scans

$$E \simeq 14.7\ \mathrm{meV},\ Q = 2.5\ \mathrm{\AA}^{-1},\ T = 6\ \mathrm{K}$$

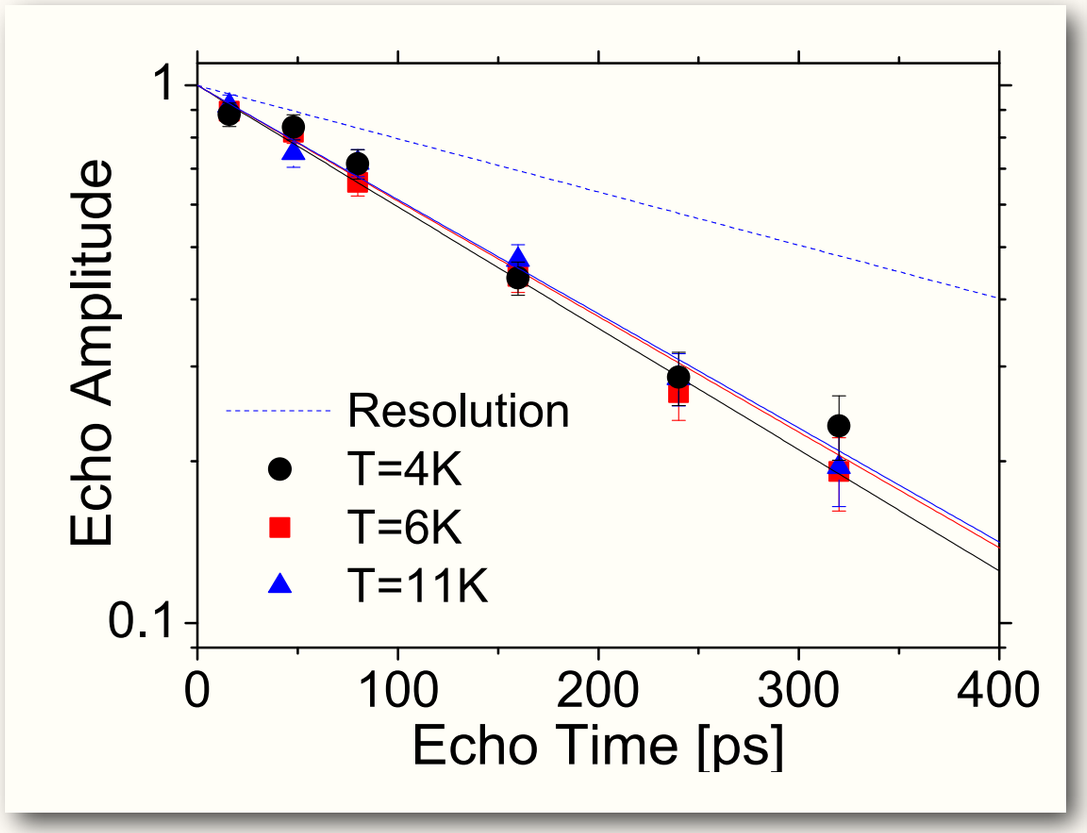


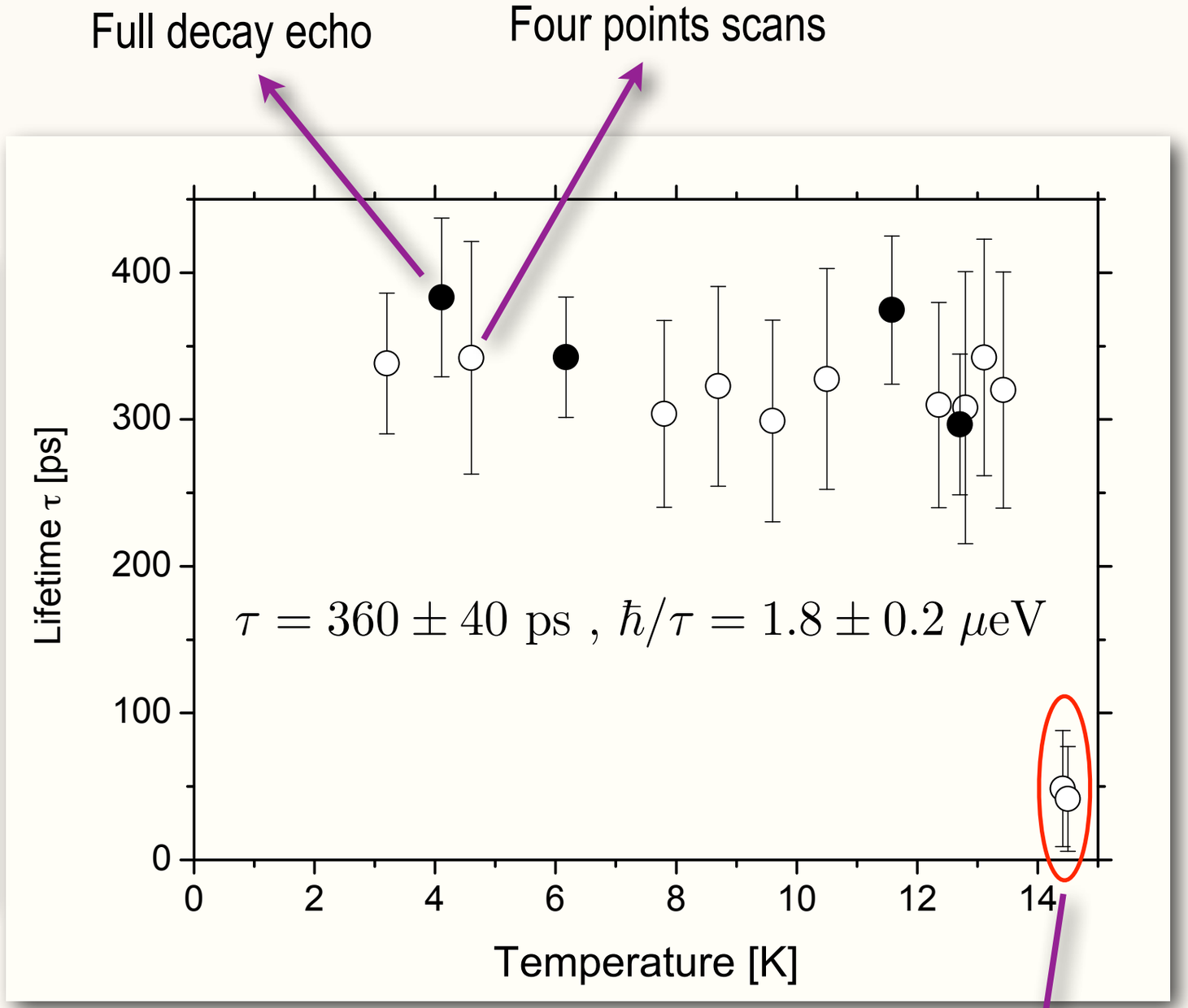


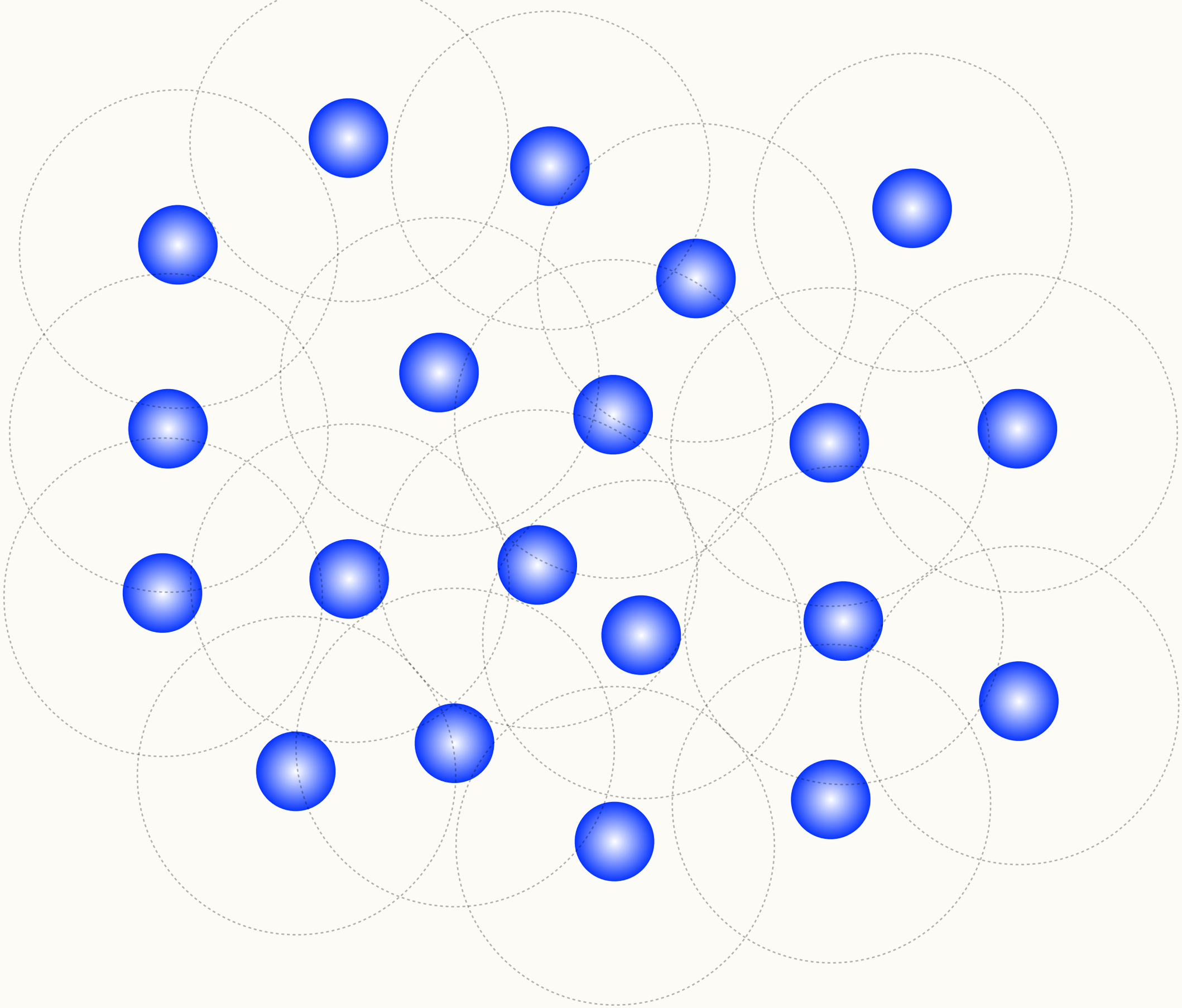


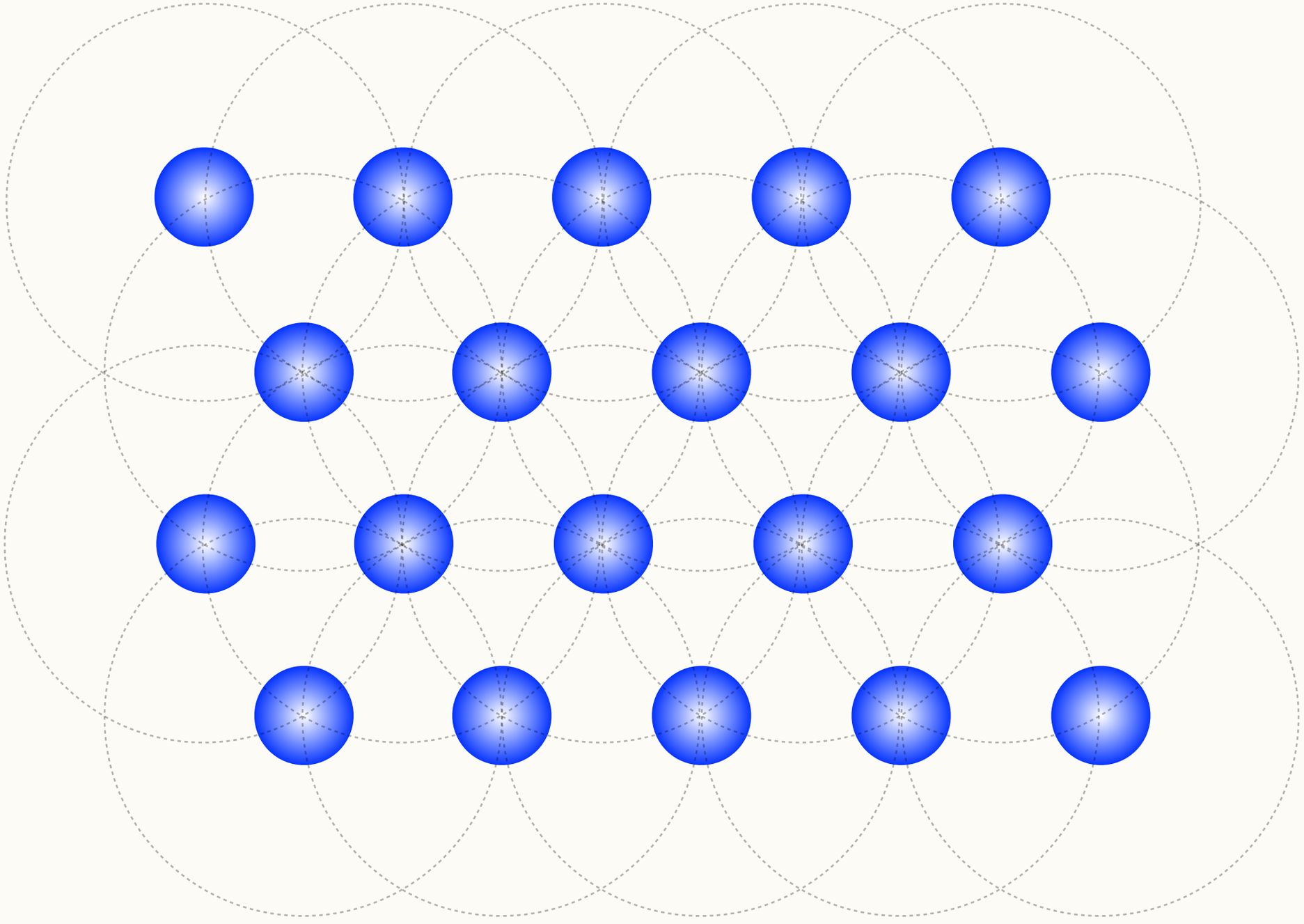
Results

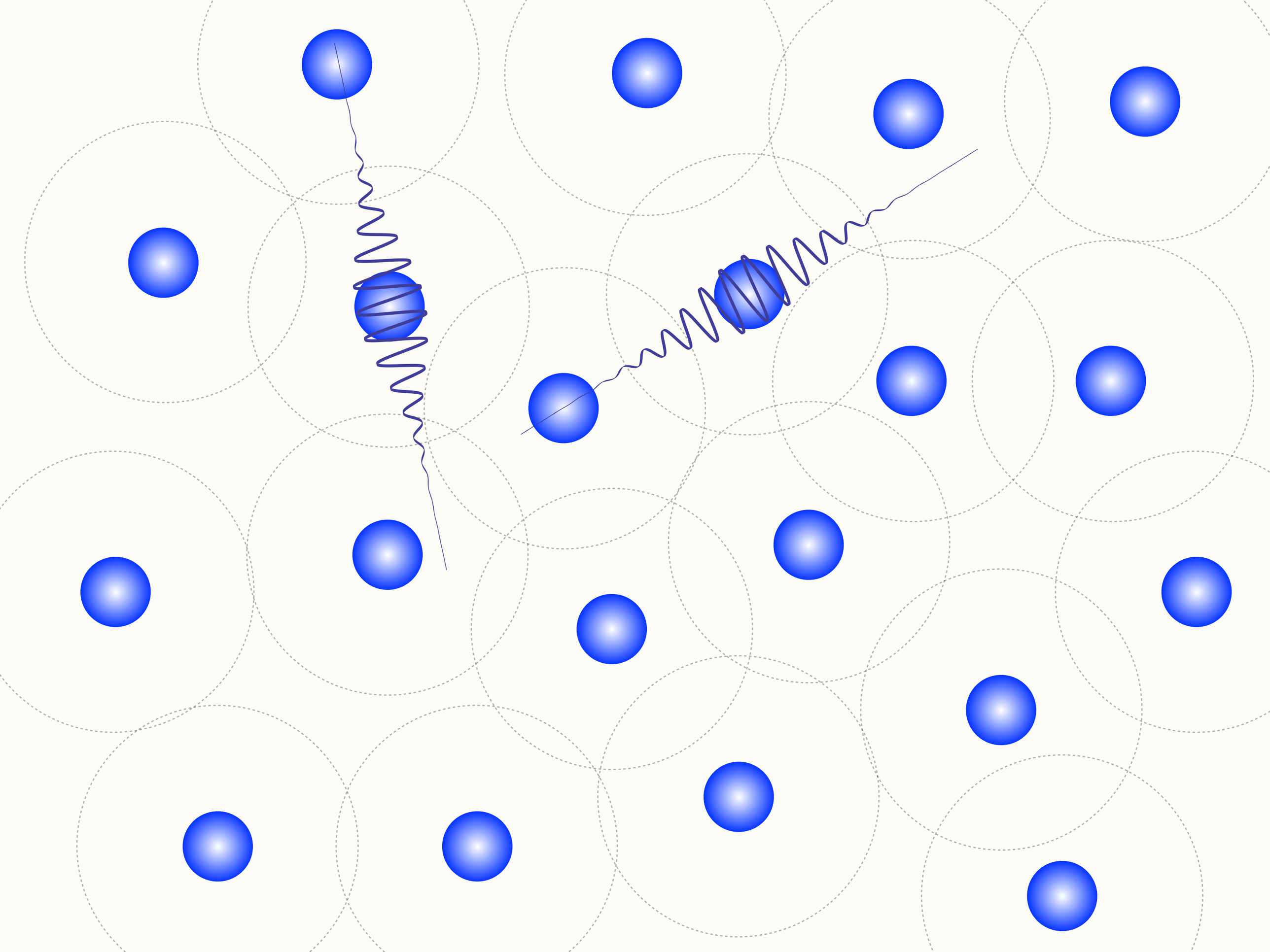
Inelastic Spin Echo

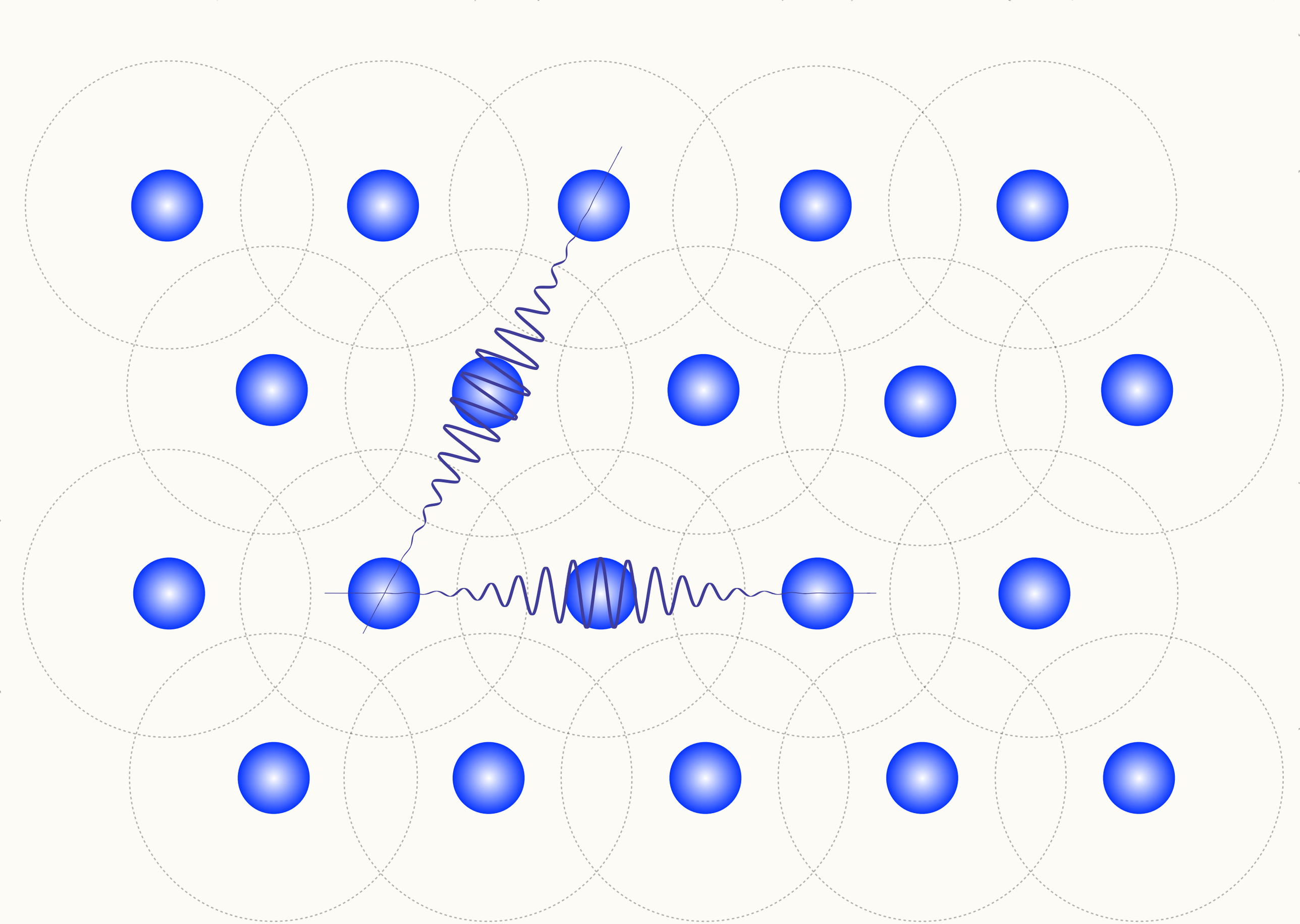












Formación en Investigación

- Becas JAE Intro (CSIC): Introducción a la investigación (5 meses prorrogables). Alumnos de los dos últimos cursos de grado

Después del grado:

- Contratos garantía juvenil (CAM)

- Acciones de Formación de Profesorado Universitario (FPU): Contratos para realizar Tesis Doctorales

- Contratos predoctorales para la formación de doctores (antiguas FPI). Contratos asociados a proyectos de investigación típicamente para realizar una tesis doctoral. En nuestro caso: posibilidad en 2023 en un proyecto conjunto con el Materials Physics Center en San Sebastian con base en dicho centro (METASTABLE AND ACTIVE CARBON-BASED MATERIALS FOR THE STORAGE AND MANAGEMENT OF CLEAN ENERGY – NOVEL PHYSICO-CHEMICAL STRATEGIES (MACMAT))