



H2020-MSCA ITN
Grant n. 956099



*Nan*ED



ISTITUTO ITALIANO
DI TECNOLOGIA

The NanED project

Mauro Gemmi- Istituto Italiano di Tecnologia

Welcome



Nan  **ED**

Welcome

NanED aims to train a new generation of young electron crystallographers that will transform 3D ED to a stable, standardized, widely recognized and widely applied method that can be easily implemented and used in any crystallography lab.

A total of **15 PhD** students



Day1 – Getting Together

09:15–10:15 Mauro Gemmi (IIT): **Project overview**

10:15–10:30 Giulia Zunino (IIT): **Administrative cookbook**



11:00 – 11:30 Philippe Boullay (CNRS): **Training and secondment.**

11:30 – 12:30 **ESR presentation**

12 :30–13 :00 Hongyi Xu (SU) : **Communication and dissemination strategy**



14 :30 – 15 :30 **Partner Presentation**

15 :30 – 16 :30

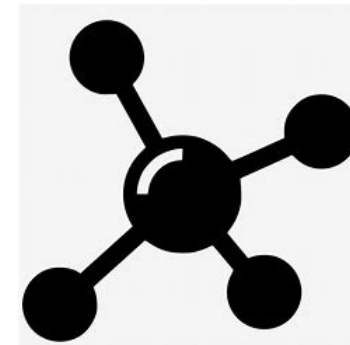
ESR meeting

Consortium meeting

16 :30-17 :00 Summary of Day1 ; Q&A time.....



Day2 – Scientific Overview



09:00–9:45 Mauro Gemmi (IIT): **WP1 – 3D ED techniques**

9:45–10:30 Xiaodong Zou (SU): **Serial 3D ED**



10:45–11:30 Lukas Palatinus (FZU): **WP3 – Precise electron crystallography**

11:30-12:15 Joke Hadermann (UA): **In-situ 3D ED**

12:15-13:00 Ute Kolb (JGU): **3D ED on defective materials**



14:00 – 14:45 Jan Pieter Abrahams (UBA): **WP2 – 3D ED on macromolecules**

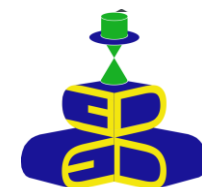
14:45 – 15:30 Hongyi Xu (SU): **Structure-based drug discovery by 3D ED**

15:30 – 16:15 Ute Kaiser (UULM): **WP4 – Electron crystallography of 2D materials**



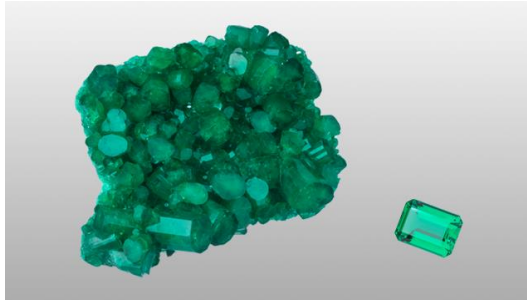
16:45 – 17:30 Philippe Boullay (CNRS): **3D ED on nanomaterials**

17:30 - 18:15 Cheuk-Wai Tai (SU): **Electron PDF studies**



What is all about?

Natural or synthetic
unknown crystal

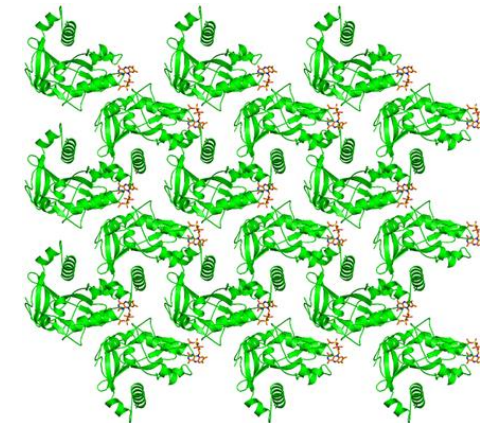
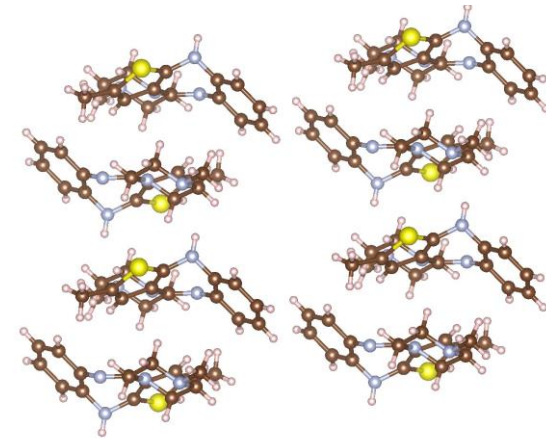
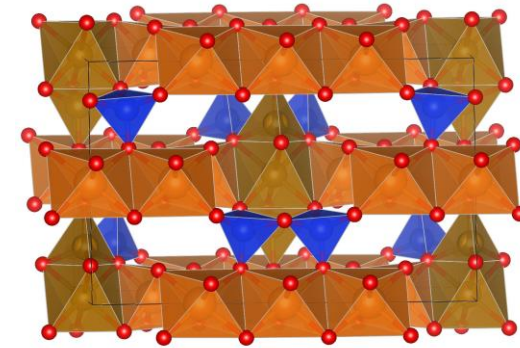


THE CRYSTALLOGRAPHIC PROBLEM

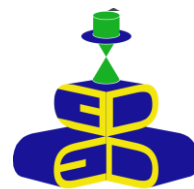
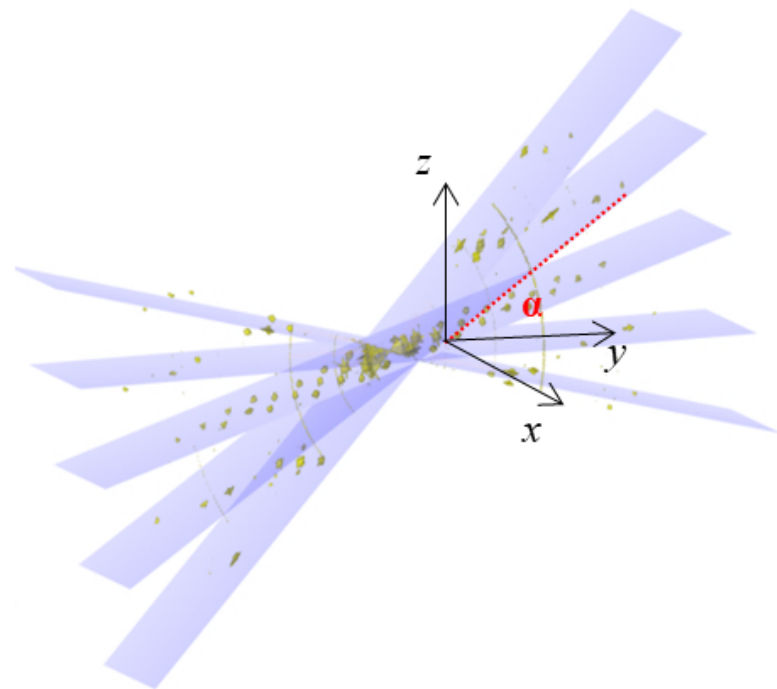
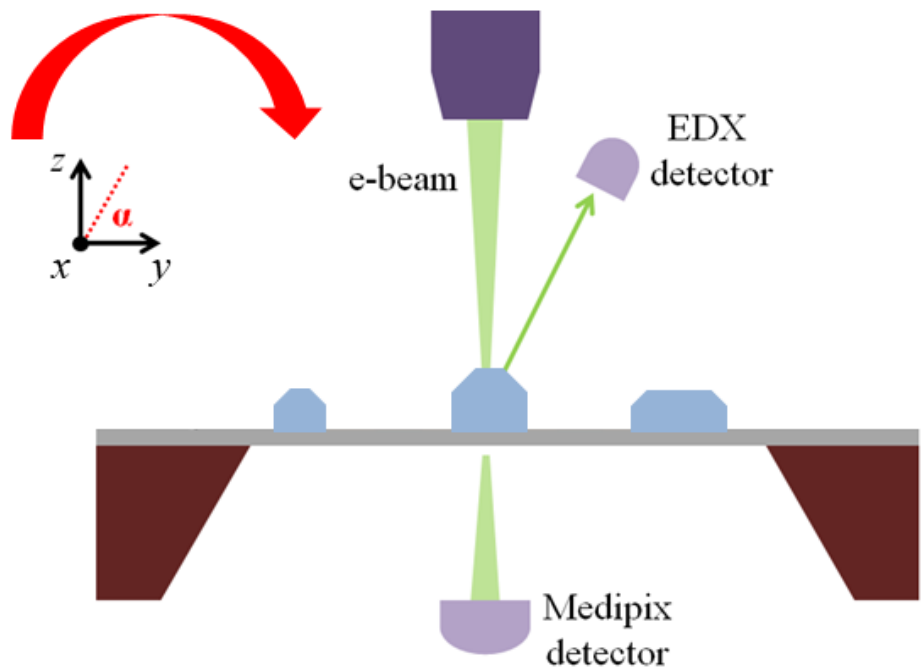


Having a minimal knowledge:
Tentative chemical composition
Maybe we have the molecule.....

When the crystals get nano!!!!

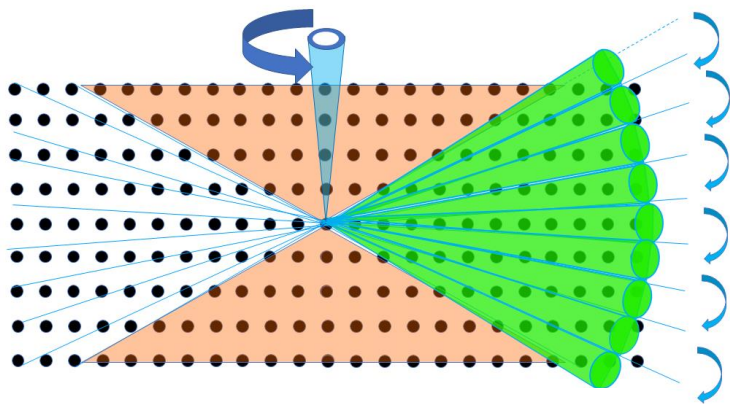


3D ED



Scientific Objectives

Establish optimised and portable sample preparation, data collection and data reduction strategies for 3D ED experiments

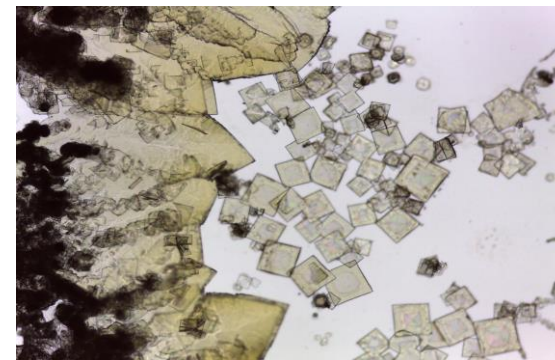


The technique

Enhanced refinement procedures for nanostructures.



Ab-initio methods for structure solution of macromolecules.

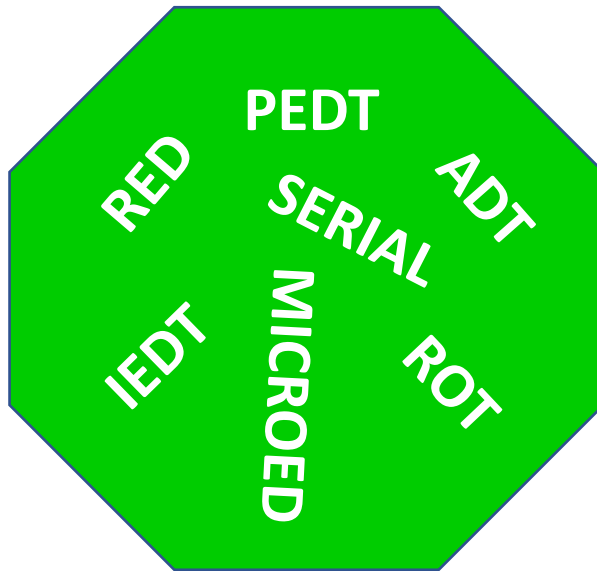


The materials

Road map to nano.

The technique

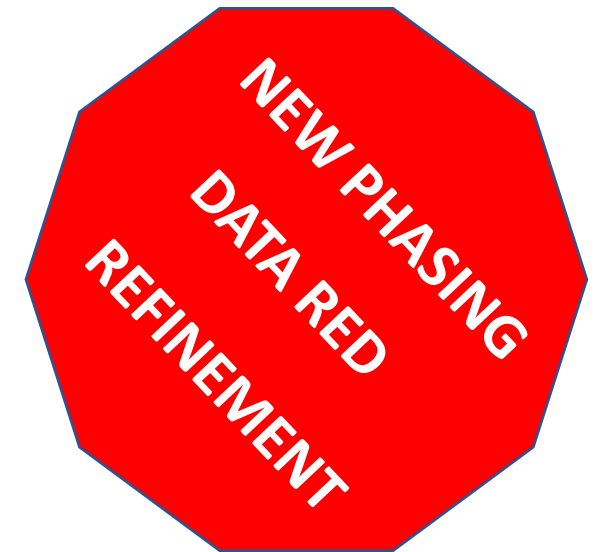
The proper recipe for any sample



SELECT



TEST



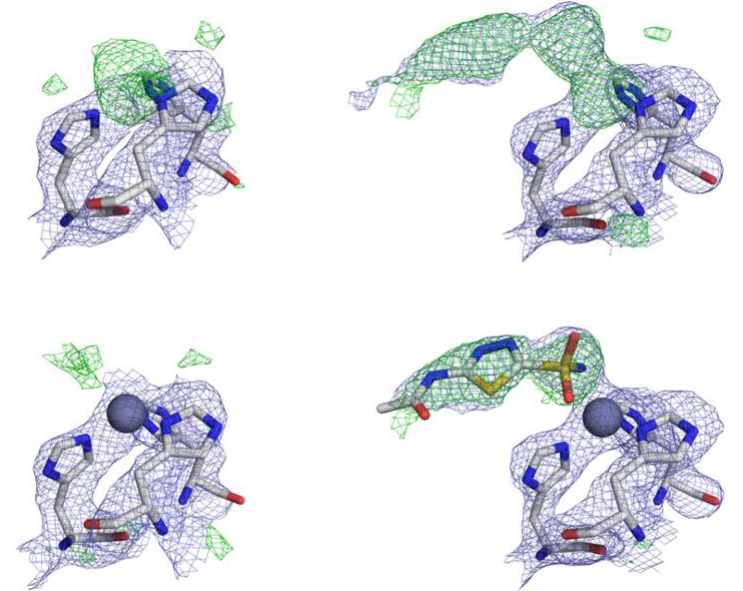
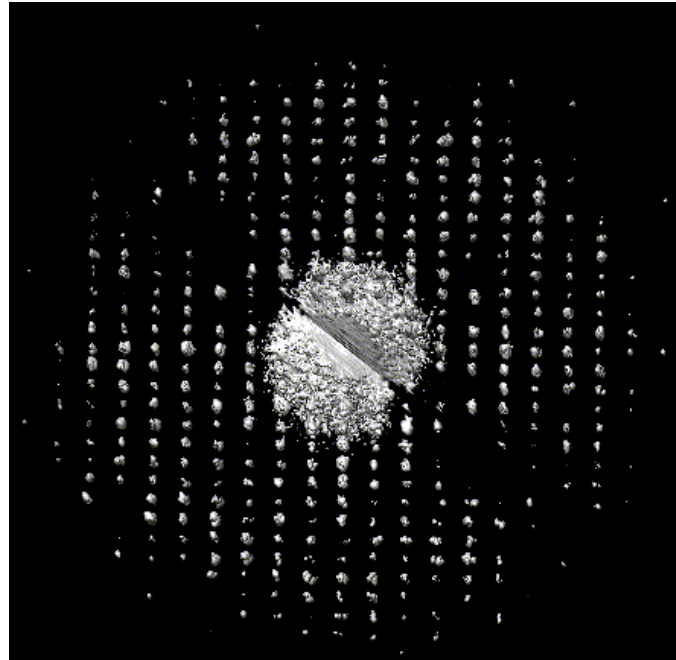
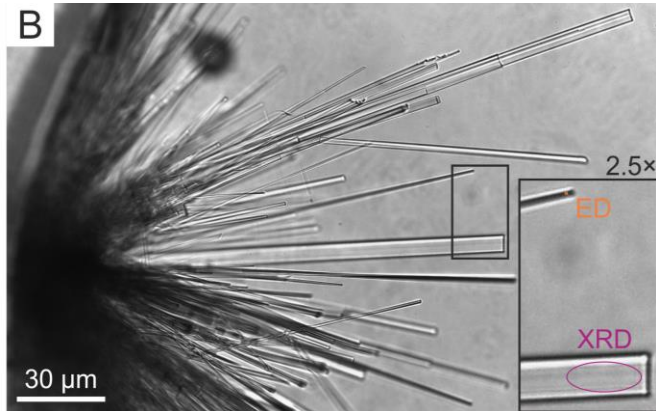
ANALYZE

This is what will give expertises to our student to spend



The materials

Ab-initio methods for structure solution of macromolecules.



**VERY VERY
CHALLENGING !**

Can we phase ab-initio 3D ED on proteins?

Can we use peculiarity of 3D ED to detect charge states?

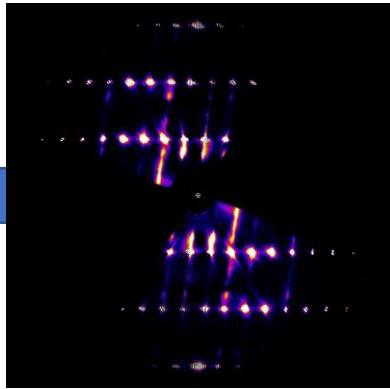
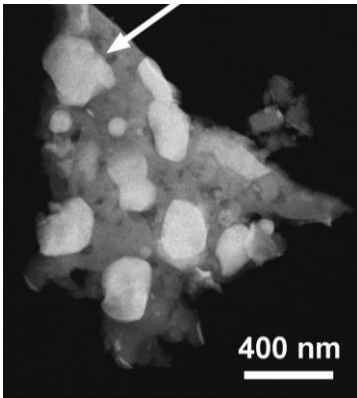
Can we use imaging for phasing?



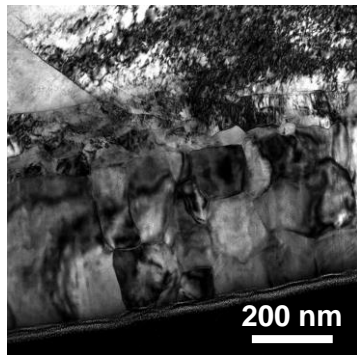
The materials

Road map to nano

Embedded

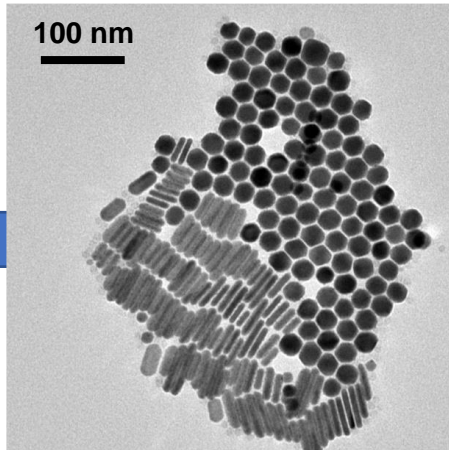


Disordered

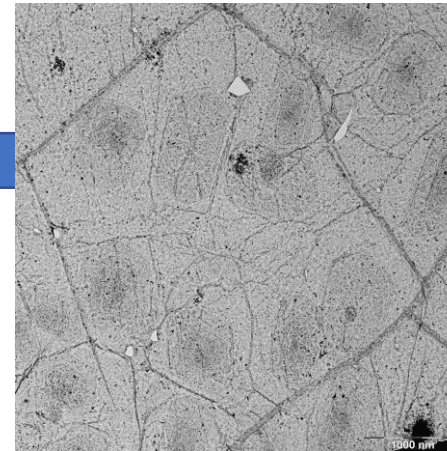
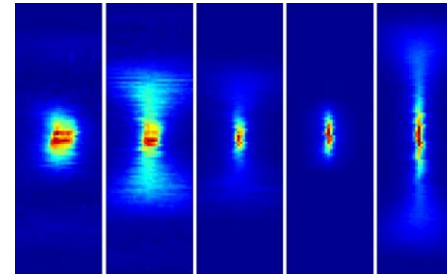


Thin films

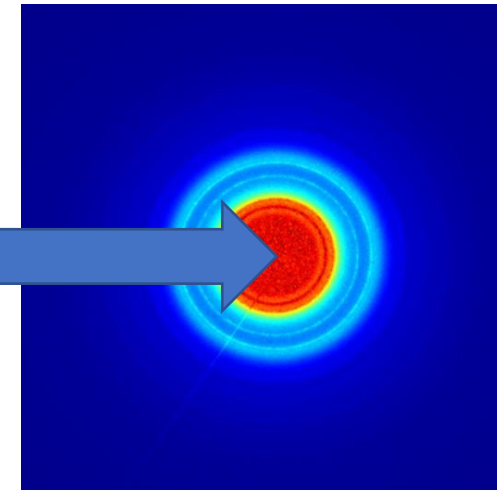
Unconventional samples



Nanoparticles



2D Materials



Amorphous

E-PDF

Minimum crystal size ?
Diffraction with nanobeams

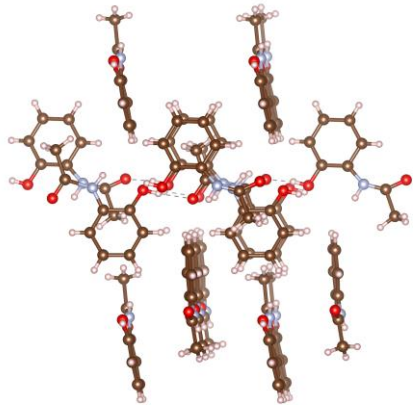
Are small crystals the same as bulk?



Project scientific implementation

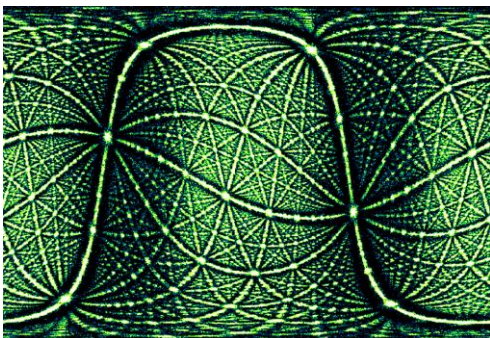
Workpackages

WP1 Beam and vacuum sensitive materials



IIT

WP3 Accurate crystallography of complex nanomaterials



FZU

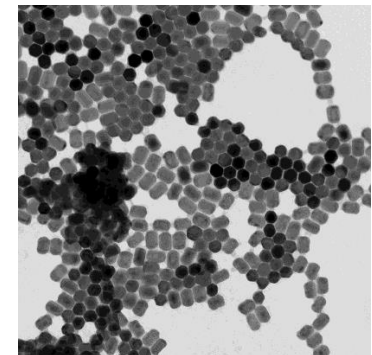


WP2 Electron crystallography for life science



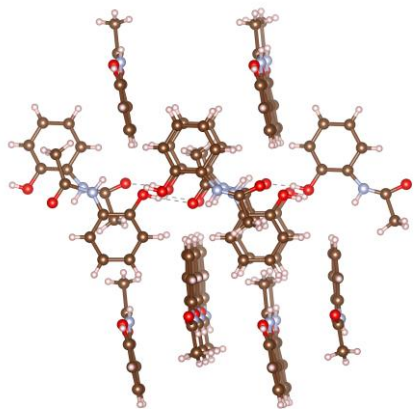
UBA

WP4 Crystallography beyond nanocrystals



UULM





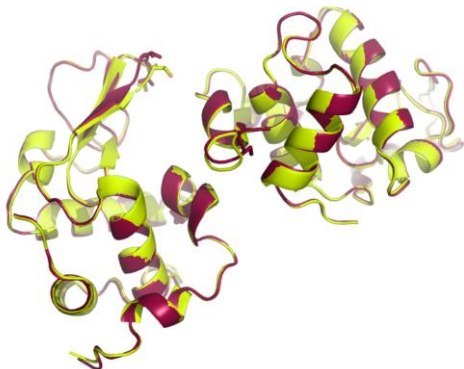
WP1 Beam and vacuum sensitive materials

IIT

WP1 aims at the setting-up of sample preparation, data acquisition and data reduction strategies for an efficient structure characterisation of beam and vacuum sensitive materials.

- ☐ Fast and low dose data collection
- ☐ Fast crystal search strategies
- ☐ Special strategies of sample preparation to protect beam and vacuum sensitive samples

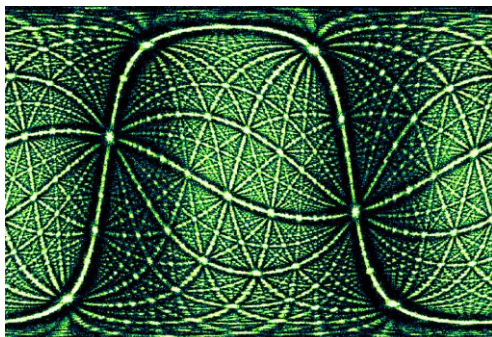




WP2 Electron crystallography for life science

UBA

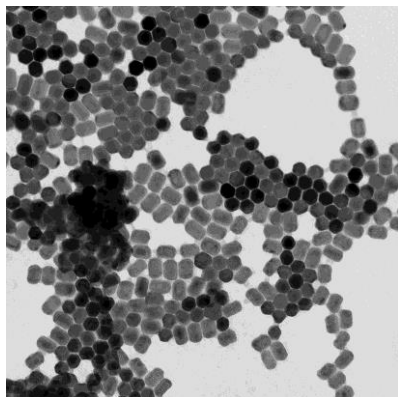
WP2 is devoted to the development of both the experimental procedures and ab-initio structure solution methods for the investigation of macromolecular nanocrystals.



WP3 Accurate crystallography of complex nanomaterials

FZU

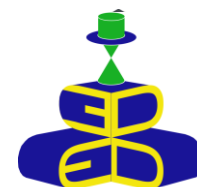
In WP3 accuracy and precision of structure refinement will be pushed in order to be fully comparable with x-ray diffraction methods.



WP4 Crystallography beyond nanocrystals

UULM

WP4 aims to expand the applicability of 3D ED to complex nanomaterials that cannot be considered properly crystalline.



Management Workpackages



WP5 ESR networking and training activity

CNRS

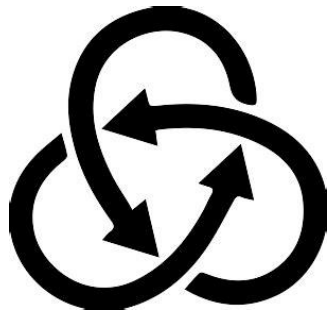
WP5 is devoted to organize, coordinate, control and supervise the network training activities.



WP6 Dissemination, communication and exploitation

SU

WP6 aims to ensure the proper communication and dissemination of project outcomes to different target audiences and to guarantee appropriate protection measures to ensure exploitation



WP7 Project management

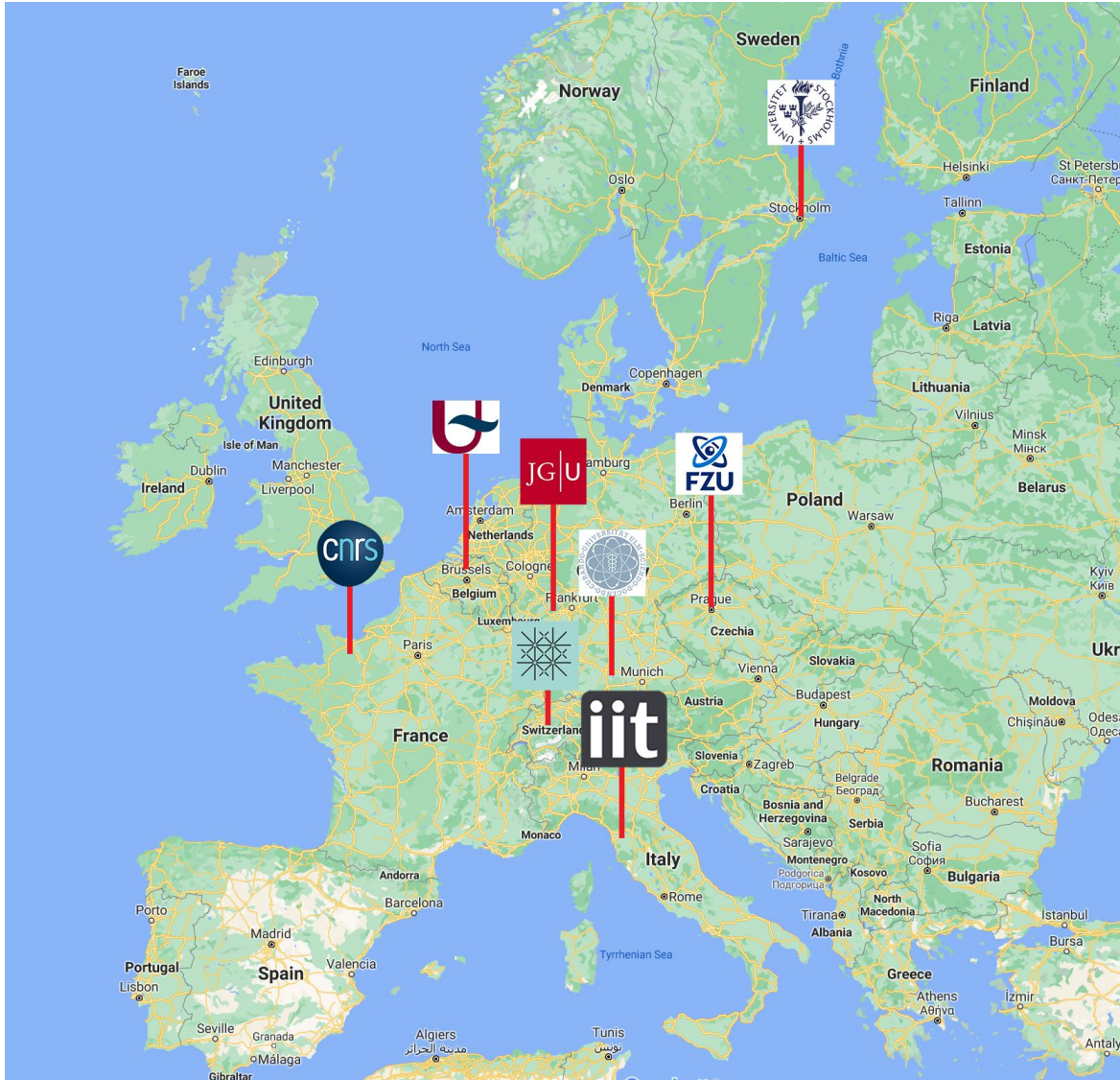
IIT

WP7 aims to ensure an efficient project execution leading to the achievement of NanED's objectives

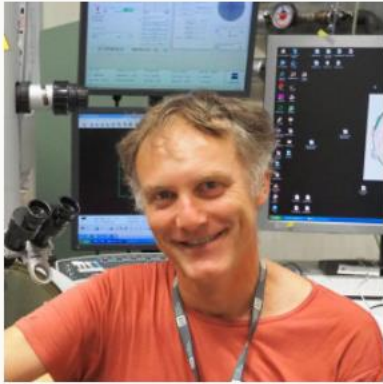




The team



The team



Mauro Gemmi
Project Coordinator and WP1/7
leader



Jan Pieter Abrahams
WP2 leader



Philippe Boullay
WP5 leader



Xiaodong Zou
WP6 leader



Joke Hadermann



Ute Kaiser
WP4 Leader



Ute Kolb



Lukas Palatinus



Cheuk-Wai Tai



Hongyi Xu





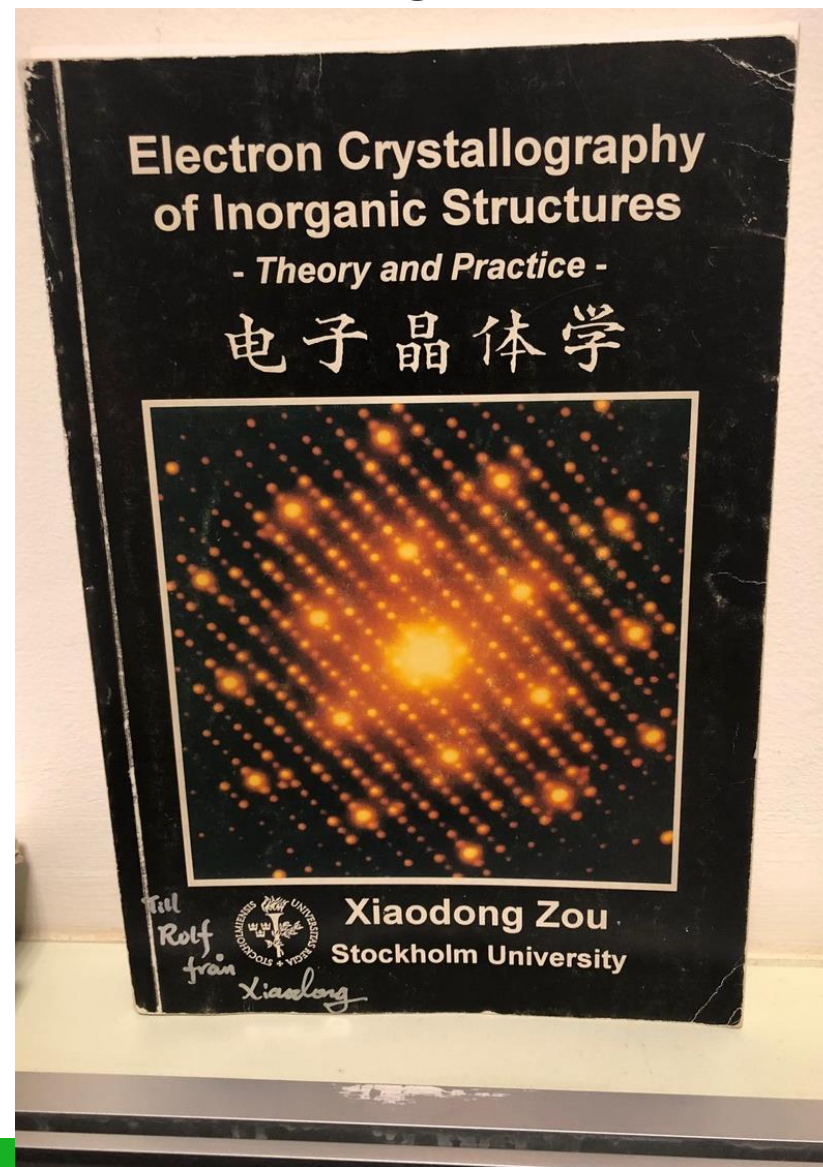
Xiaodong Zou

She is a pioneer of the structure solution using electron data

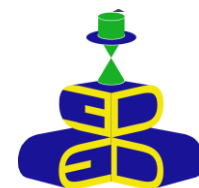


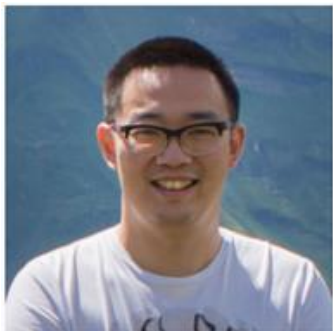
Stockholm University

Xiaodong Zou
WP6 leader



Arrheniuslaboratoriet





Hongyi Xu

SCIENCE ADVANCES | RESEARCH ARTICLE

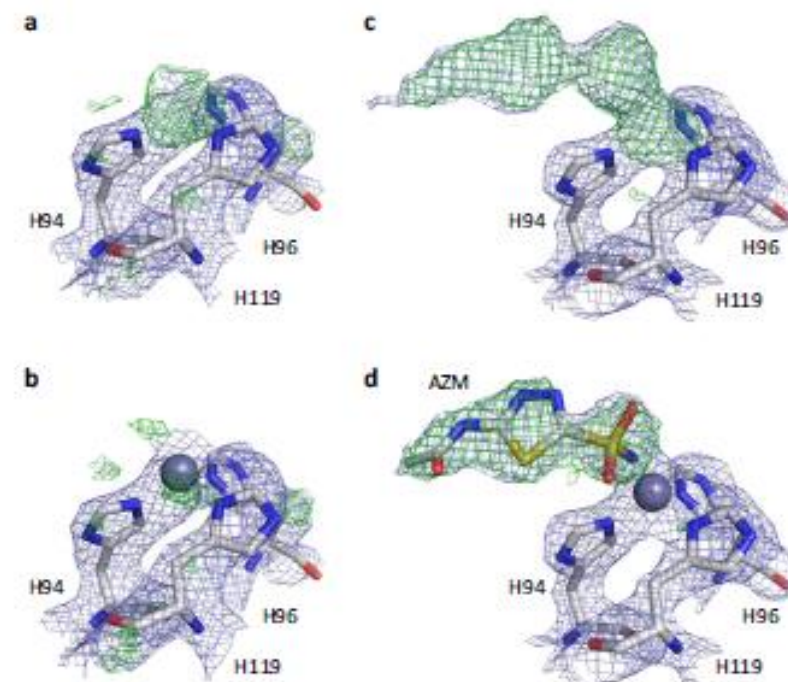
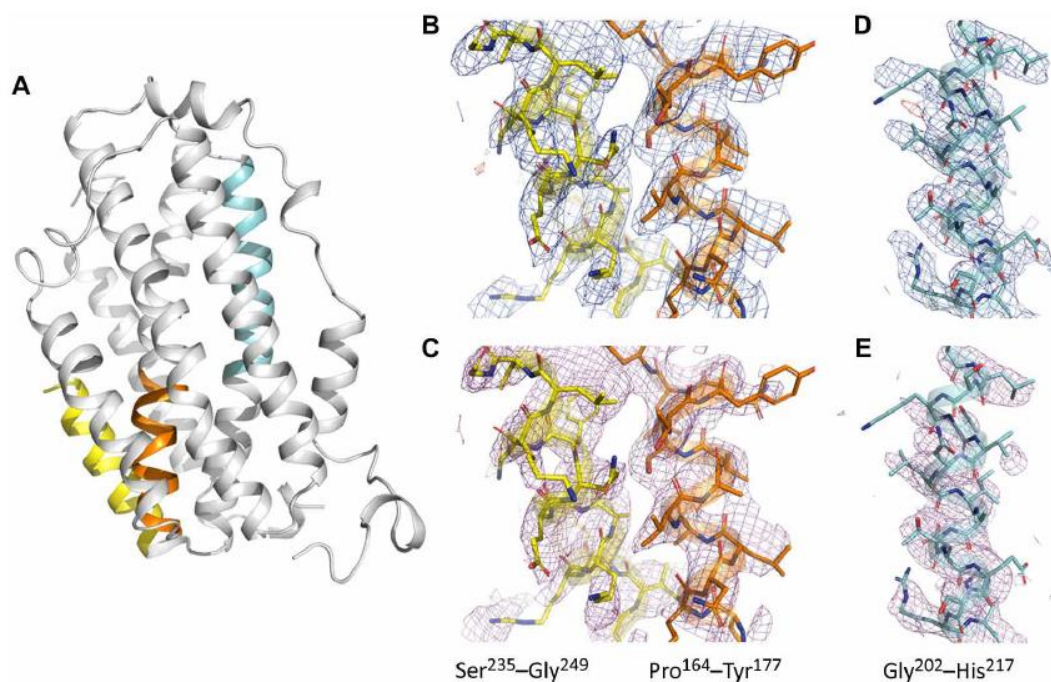
STRUCTURAL BIOLOGY

Solving a new R2lox protein structure by microcrystal electron diffraction

Hongyi Xu^{1*†}, Hugo Lebrette^{2†}, Max T. B. Clabbers^{1†}, Jingjing Zhao¹, Julia J. Griesse^{2,3}, Xiaodong Zou^{1*}, Martin Högbom^{2*}

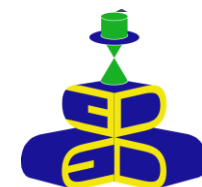
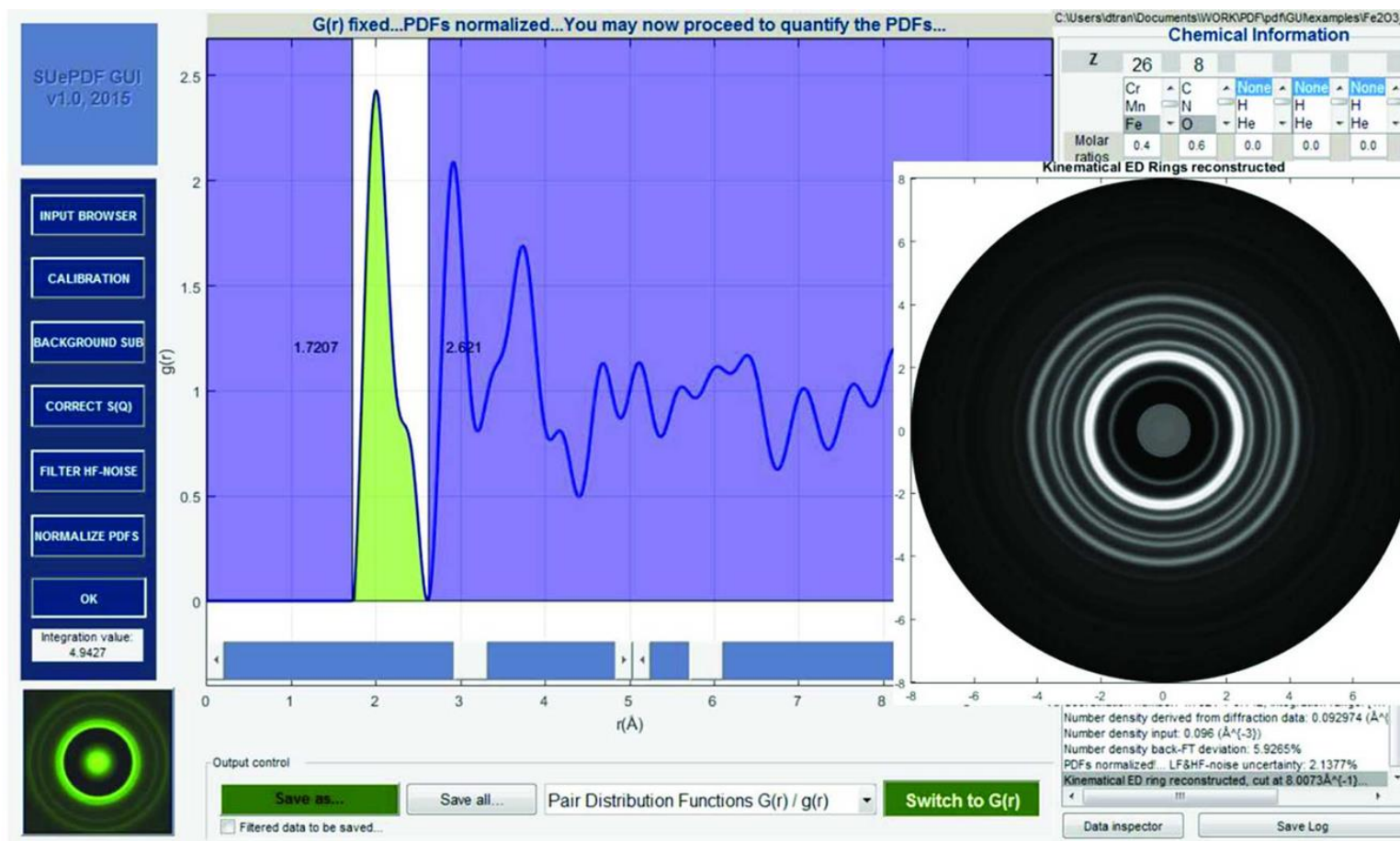


Stockholm
University





Cheuk-Wai Tai





Joke Hadermann



NANO LETTERS

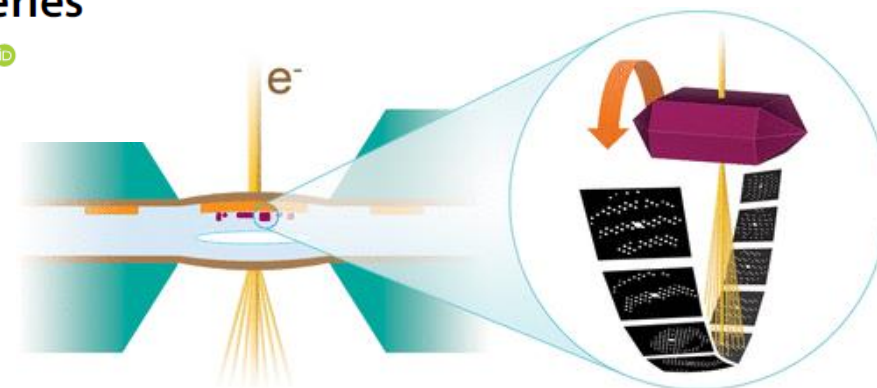
Cite This: *Nano Lett.* 2018, 18, 6286–6291

Letter

pubs.acs.org/NanoLett

In Situ Electron Diffraction Tomography Using a Liquid-Electrochemical Transmission Electron Microscopy Cell for Crystal Structure Determination of Cathode Materials for Li-Ion batteries

Olesia M. Karakulina,[†] Arnaud Demortière,^{*,‡,§} Walid Dachraoui,[§] Artem M. Abakumov,^{||} and Joke Hadermann^{*,†}





Philippe Boullay

Inorganic Chemistry

Article

pubs.acs.org/IC



Precession Electron Diffraction Tomography for Solving Complex Modulated Structures: the Case of $\text{Bi}_5\text{Nb}_3\text{O}_{15}$

Philippe Boullay,^{*,†} Lukas Palatinus,[‡] and Nicolas Barrier[†]



JOURNAL OF
APPLIED
CRYSTALLOGRAPHY

ISSN 1600-5767

Precession electron diffraction tomography on twinned crystals: application to CaTiO_3 thin films

Gwladys Steciuk,^{a,b} Adrian David,^a Václav Petříček,^b Lukáš Palatinus,^b Bernard Mercey,^a Wilfrid Prellier,^a Alain Pautrat^a and Philippe Boullay^{a*}

NANO LETTERS

Letter

Cite This: *Nano Lett.* 2017, 17, 6575-6582

pubs.acs.org/NanoLett

Novel Layered Supercell Structure from $\text{Bi}_2\text{AlMnO}_6$ for Multifunctionalities

Leigang Li,^{†,‡} Philippe Boullay,^{§,∇} Ping Lu,^{||} Xuejing Wang,[†] Jie Jian,[†] Jijie Huang,[†] Xingyao Gao,[†] Shikhar Misra,[†] Wenrui Zhang,^{‡,¶} Olivier Perez,[§] Gwladys Steciuk,[§] Aiping Chen,^{⊥,¶} Xinghang Zhang,[†] and Haiyan Wang^{*,†,‡,‡,¶}





Lukas Palatinus


PETS

Pets 2.0 [C:\Users\mgemmi\OneDrive - Fondazione Istituto Italiano Tecnologia\PREVIOUS\Documents\RICERCA\Iryna\Arcniegas\TMA\renamed\Copia_09Gemmi.pts]

File Edit View Help

Parameters	
Peak search	
Rotation axis	
Peak analysis	
Find unit cell and orientation matrix	
Process frames for integration	
Optimize geometry and integration parameters	
Finalize integration	
Generate a 3D map	
Reciprocal-space sections	
Write check files	

T A
Č R

 **FZU**

Institute of Physics
of the Czech
Academy of Sciences


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value 17.570; scale 1.25121
Final values of the parameter:
Optimized omega: 17.562
Finished reading 1554 peaks from the file Copia_09Gemmi
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
Jana


Jana2006


File Edit/View Run Wizards Parameters Tools


 Edit M50


 Edit atoms


 Edit profile


 Structure solution


 Fourier


 Contour


 Refine


 Dist

 Matrix calculator

 Plot structure

 Profile viewer

 Graph

 SetCommands

Structure: C:\Data\EDT\Iryna\symmetry\jana\prova4



Fyzikální ústav Akademie
věd České republiky



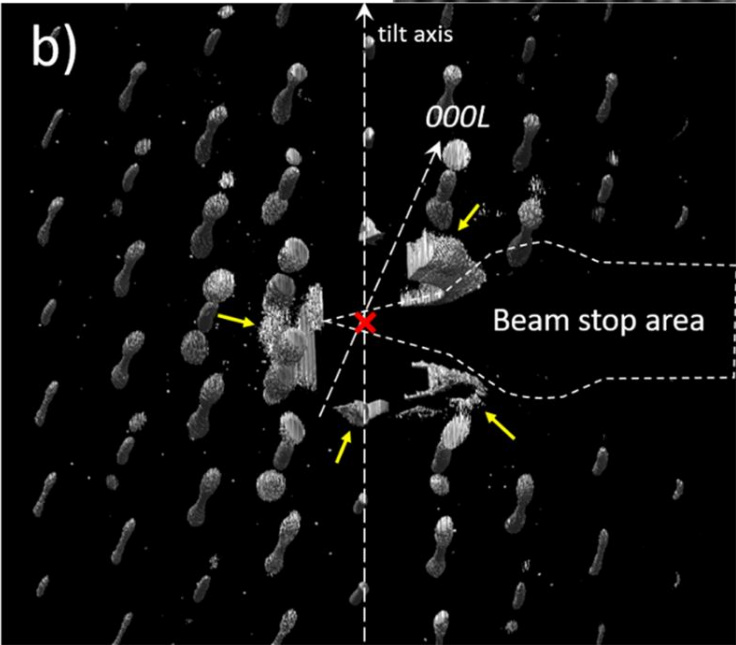
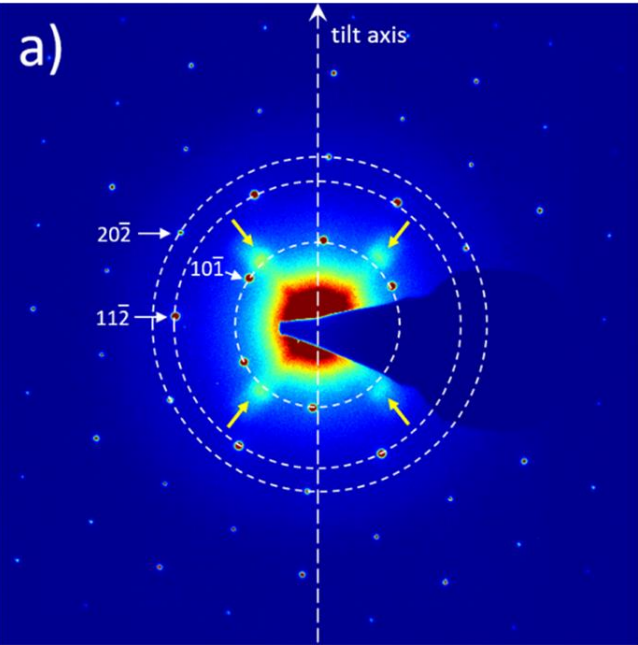
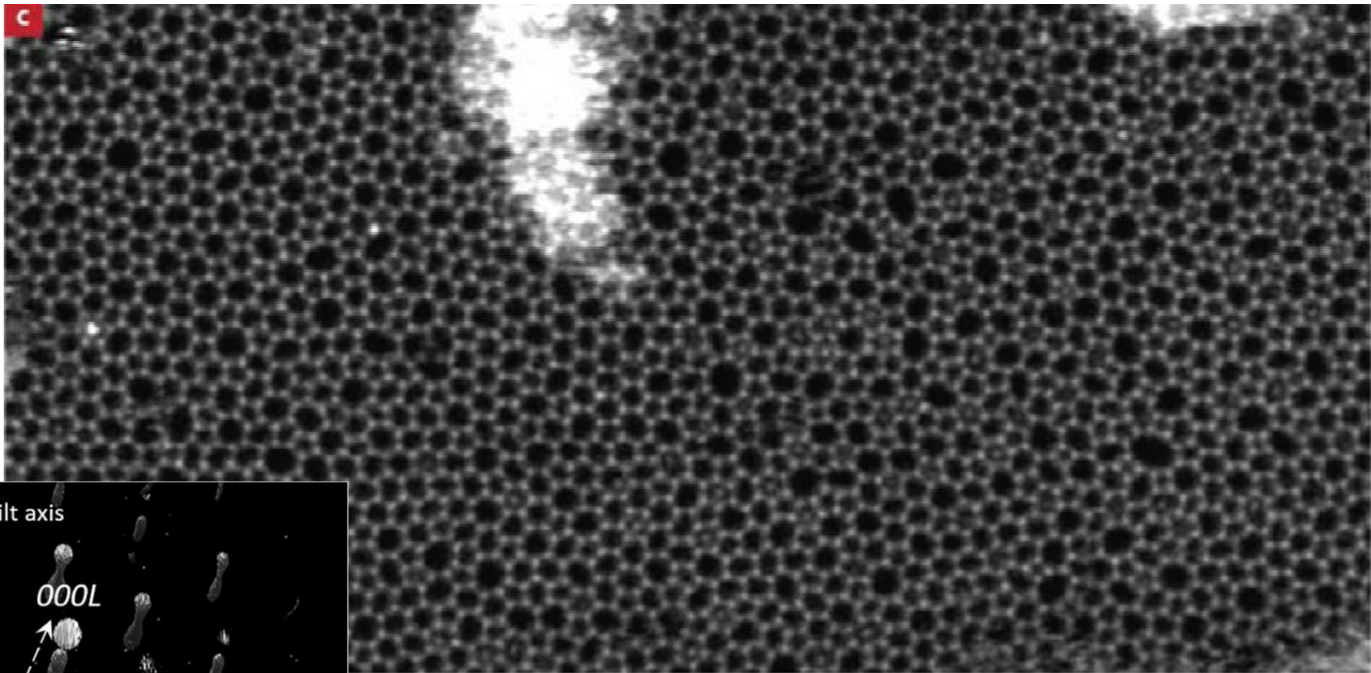
Ute Kaiser



Tatiana Gorelik



She is directing the **SALVE** project for low-voltage aberration-corrected electron microscope enabling sub-Angstrom resolution





Jan Pieter Abrahams



Acta Crystallographica Section D
**Biological
Crystallography**
ISSN 0907-4449

A Medipix quantum area detector allows rotation electron diffraction data collection from submicrometre three-dimensional protein crystals

**Igor Nederlof, Eric van
Genderen, Yao-Wang Li and
Jan Pieter Abrahams***

When protein crystals are submicrometre-sized, X-ray radiation damage precludes conventional diffraction data collection. For crystals that are of the order of 100 nm in size, at best only single-shot diffraction patterns can be collected

Received 18 April 2012
Accepted 9 April 2013





Ute Kolb



Available online at www.sciencedirect.com



Ultramicroscopy 107 (2007) 507–513

ultramicroscopy

www.elsevier.com/locate/ultramic



Towards automated diffraction tomography: Part I—Data acquisition

U. Kolb^{a,*}, T. Gorelik^a, C. Kübel^b, M.T. Otten^c, D. Hubert^c

Ultramicroscopy 109 (2009) 758–765



Contents lists available at ScienceDirect

Ultramicroscopy

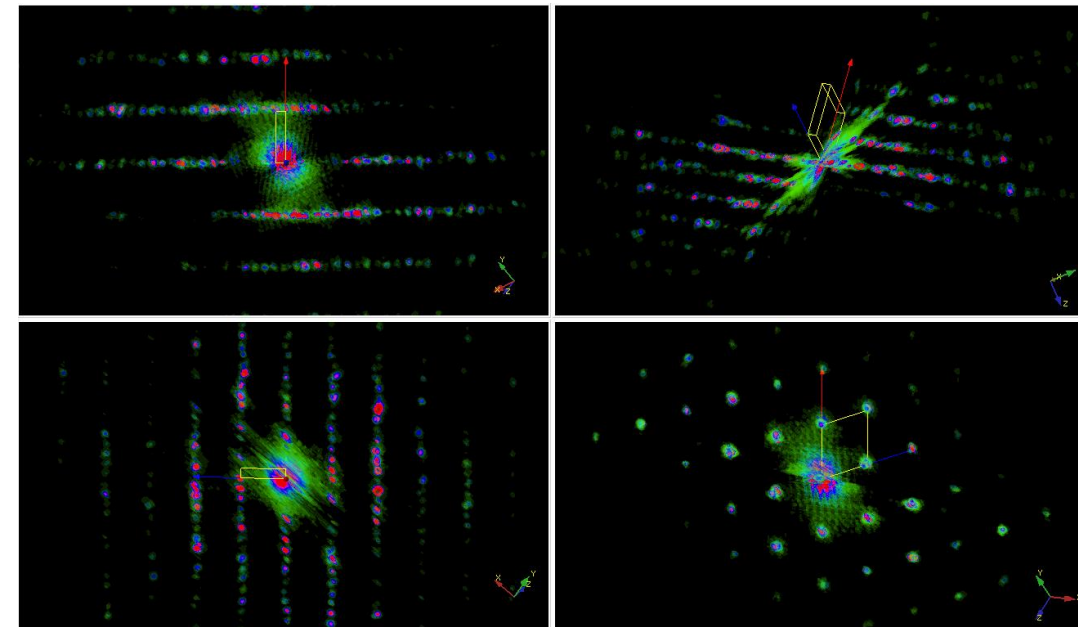
journal homepage: www.elsevier.com/locate/ultramic



ADT3D

“Ab initio” structure solution from electron diffraction data obtained by a combination of automated diffraction tomography and precession technique

E. Mugnaioli, T. Gorelik, U. Kolb *





Mauro Gemmi



Ultramicroscopy 84 (2000) 133–142

ultramicroscopy

www.elsevier.nl/locate/ultramic



ISTITUTO ITALIANO
DI TECNOLOGIA

Structure determination of ϕ -Bi₈Pb₅O₁₇ by electron and powder X-ray diffraction

M. Gemmi^{a,b}, L. Righi^c, G. Calestani^c, A. Migliori^{a,*}, A. Speghini^d,
M. Santarosa^d, M. Bettinelli^d

Acta Crystallographica Section A
**Foundations of
Crystallography**

ISSN 0108-7673

Received 19 July 2002
Accepted 6 December 2002

Structure of Ti₂P solved by three-dimensional electron diffraction data collected with the precession technique and high-resolution electron microscopy

Mauro Gemmi,^{a,*†} Xiaodong Zou,^a Sven Hovmöller,^a Andrea Migliori,^b Marie Vennström^c and Yvonne Andersson^c



JOURNAL OF
APPLIED
CRYSTALLOGRAPHY

ISSN 1600-5767

Fast electron diffraction tomography

Mauro Gemmi,^{a,*} Maria G. I. La Placa,^a Athanassios S. Galanis,^b Edgar F. Rauch^c
and Stavros Nicolopoulos^b



Training

Local

Local training program

at the hosting institutions enrollment in a PhD program, direct research in the labs, local courses at the universities

Network

Network training program

through the participation to workshop events organized by NanED where experts both internal and external to the network will provide seminars and lectures on both technical and transferrable skills

Move

Secondment training program:

where the ERS will spend time:

- i) in other beneficiaries of the network
- ii) in partner organizations



Our partners



Companies

Synthesis

AstraZeneca

AstraZeneca

BASF
We create chemistry

BASF SE

CODEX
INTERNATIONAL

CODEX International

Roche

Roche

Instruments

AS AMSTERDAM
SCIENTIFIC
INSTRUMENTS

Amsterdam Scientific
Instruments

DENS
solutions

DENSsolutions

ELDIGO
SCIENTIFIC

ELDICO Scientific



Rigaku

NanoMEGAS
Advanced Tools for electron diffraction

NanoMEGAS

TESCAN
PERFORMANCE IN NANOSPACE

TESCAN ORSAY HOLDING

ThermoFisher
SCIENTIFIC

Thermo Fisher Scientific

Large scale facilities



Science and
Technology
Facilities Council

United Kingdom Research
and Innovation



Elettra Sincrotrone Trieste

Elettra – Sincrotrone Trieste



Diamond Light source

Universities



**UNIVERSITÀ
DI PARMA**

Università di Parma



**UNIVERZITA
KARLOVA**

Univerzita Karlova

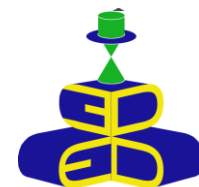
IUCr
a ruler in
crystallography



International Union of
Crystallography



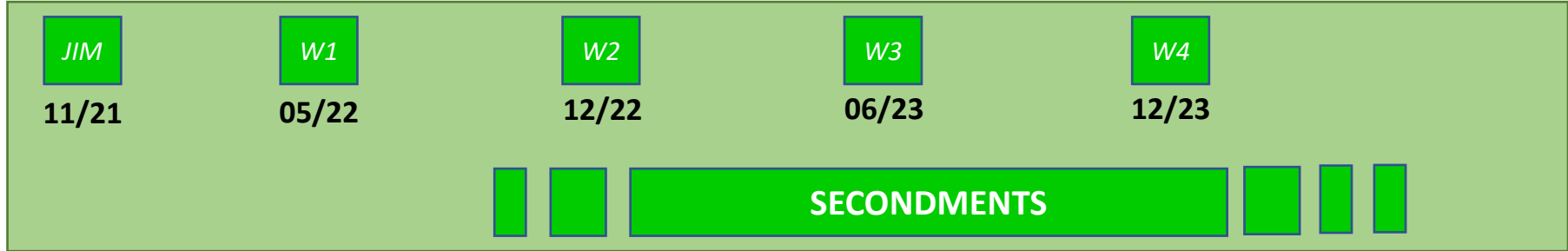
ESR	Supervisory Team	
	Main Supervisor	Co-supervisors
ESR1	Gemmi (IIT)	Dalcanale(UNIPR), Nicolopoulos(NMG), Brázda (FZU), Batuk (UA), Yu(THF)
ESR2	Gemmi (IIT)	Dalcanale(UNIPR), Xu (SU), Van Genderen (UBA), Stowasser (RCH), McMahon (IUCr)
ESR3	Hadermann (UA)	Kolb (JGU), Perez (DENS), David (NU)
ESR4	Palatinus (FZU)	Boullay(CNRS), Plaisier (EST), Müller (BASF), Hadermann (UA)
ESR5	Palatinus (FZU)	Gemmi (IIT), van der Wal (TSC), Gorelik (ULM), McMahon (IUCr)
ESR6	Kaiser(ULM)	Boullay(CNRS), Abrahams (UBA), Prangsma (ASI)
ESR7	Gorelik(ULM)	Mugnaoli (IIT), Steinfeld (ELD), Zou (SU)
ESR8	Kolb (JGU)	Van Genderen (UBA), Müller (BASF), Hadermann (UA)
ESR9	Kolb (JGU)	Palatinus (FZU), Steinfeld (ELD), Boullay (CNRS), McMahon(IUCr)
ESR10	Xu(SU)	Käck (AZ), Brázda (FZU), Zhang (eBIC), Abrahams (UBA), Yu(THF)
ESR11	Zou(SU)	Waterman(STFC), Mugnaioli (IIT), Norberg (AZ), Kolb (JGU)
ESR12	Boullay (CNRS)	David (NU), Guilmeau (CNRS), Palatinus (FZU), Kolb (JGU), van der Wal (TSC)
ESR13	Boullay (CNRS)	Hadermann(UA), Kaiser(ULM), Plaisier (EST), Séguier (CDX)
ESR14	Abrahams (UBA)	Xu (SU), Prangsma (ASI), Kaiser (ULM), Zhang (eBIC)
ESR15	Abrahams (UBA)	Gemmi (IIT), Zou (SU), Waterman (STFC), Stowasser (RCH)



Project Timeline



Training



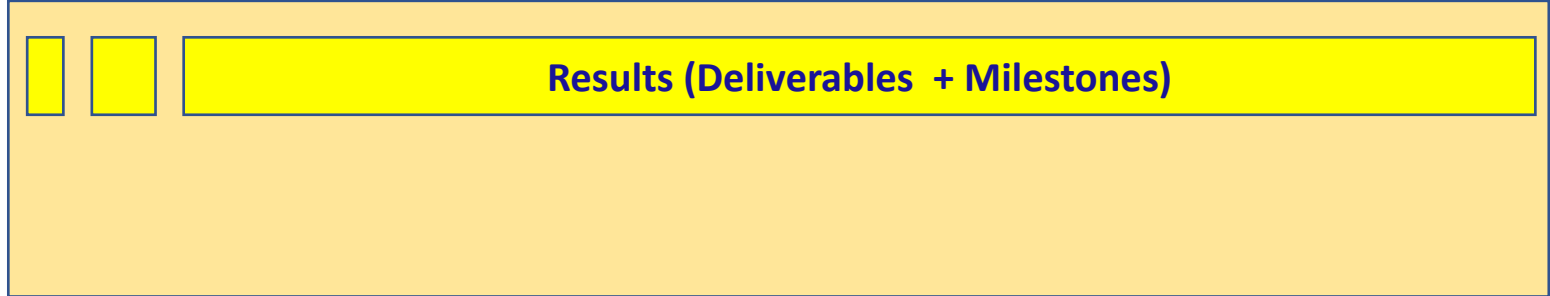
M18

M33

M39

Science

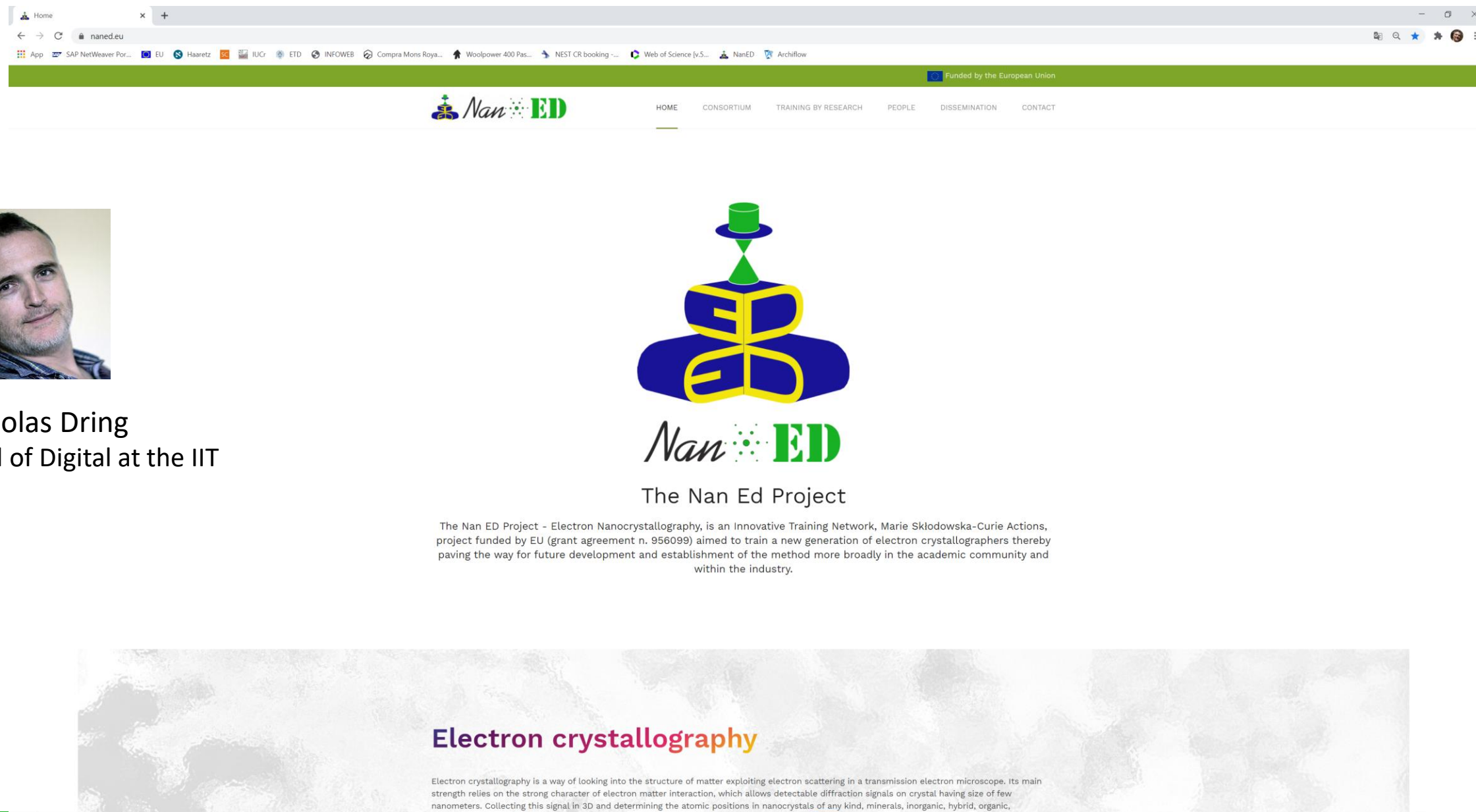
ESR Situation:
Employed 6
Selected 13
2 still missing



Website: naned.eu



Nicholas Dring
Head of Digital at the IIT



Website: naned.eu

 Funded by the European Union

[HOME](#)[CONSORTIUM](#)[TRAINING BY RESEARCH](#)[PEOPLE](#)[DISSEMINATION](#)[CONTACT](#)[OPENINGS](#)

News

PhD Students

Welcc
well a

out the Nan ED project's progress as
itional level.



NanED Ph
start @Cri

October 11, 2021

The PhD studen



Laura Gemmrich Hernandez
JGU



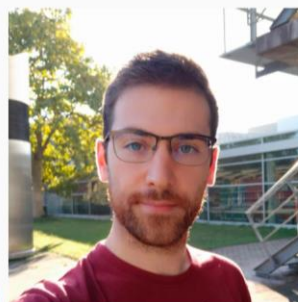
Amatassalam Ben Meriem
UB



Erica Cordero Oyonarte
CNRS



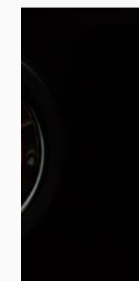
Sara Passuti
CNRS



Marco Santucci
JGU



Lei Wang
Su

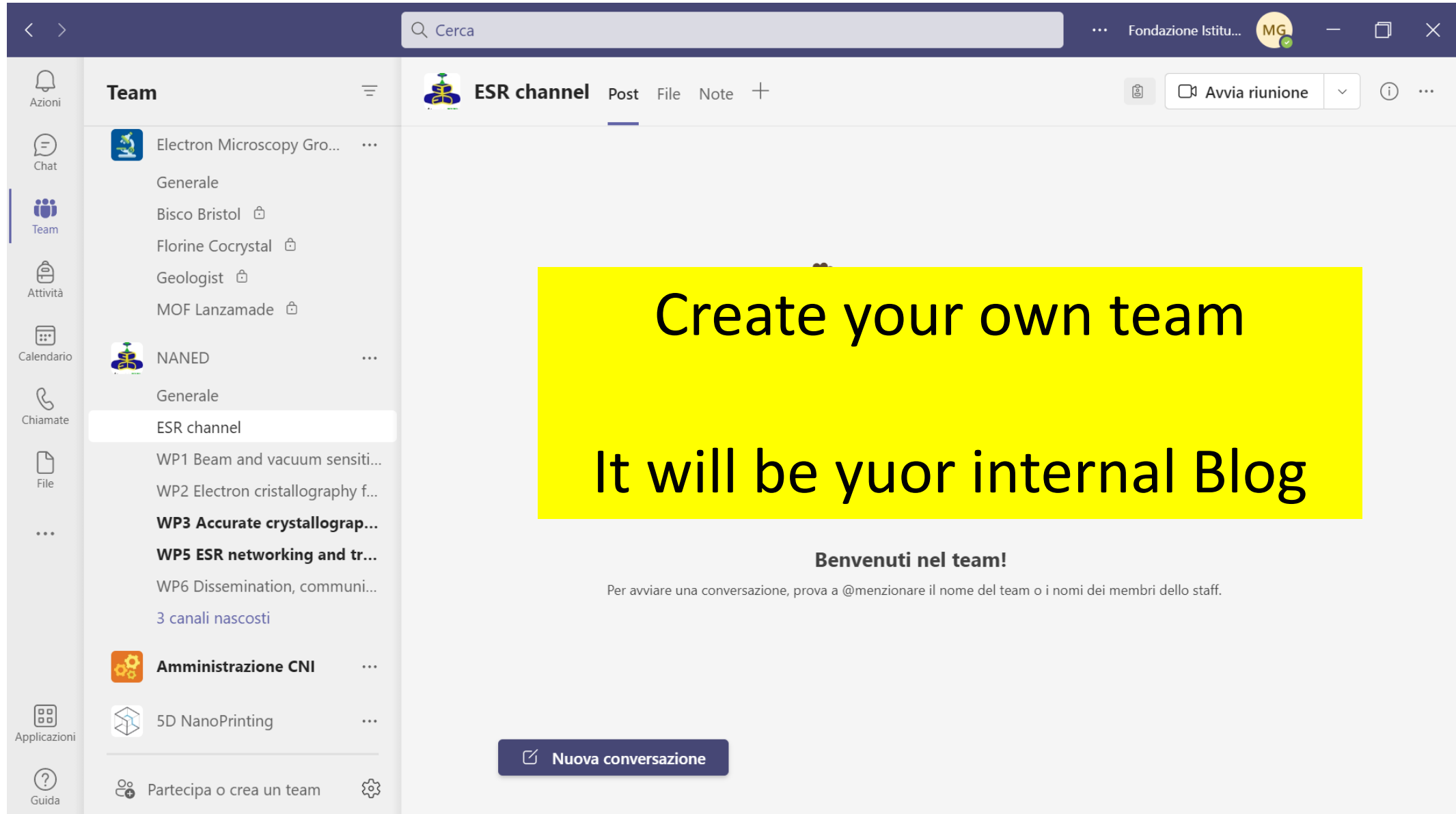


reeting

ng will take



NanED team on Teams



The screenshot displays the Microsoft Teams interface. On the left, the navigation pane shows various options: Azioni, Chat, Team (selected), Attività, Calendario, Chiamate, File, and Guida. The main pane shows the 'ESR channel' within the 'NANED' team. The channel list includes 'Generale', 'Bisco Bristol', 'Florine Cocystal', 'Geologist', 'MOF Lanzamade', and 'ESR channel' (highlighted). Below these are several work packages (WP1 to WP6) and a link to '3 canali nascosti'. At the bottom of the channel list, there are options for 'Amministrazione CNI' and '5D NanoPrinting'. A large yellow box is overlaid on the channel content with the text 'Create your own team' and 'It will be your internal Blog'. Below the box, a welcome message reads 'Benvenuti nel team!' followed by instructions on how to start a conversation. A 'Nuova conversazione' button is at the bottom.

Team

ESR channel

Post File Note +

Avvia riunione

Create your own team

It will be your internal Blog


Benvenuti nel team!

Per avviare una conversazione, prova a @menzionare il nome del team o i nomi dei membri dello staff.

Nuova conversazione




Twitter: @NanedP




- Home
- Explore
- Notifications
- Messages
- Bookmarks
- Lists
- Profile
- More

Tweet



Naned_project
37 Tweets



Naned_project
@NanedP

The Nan ED Project - Electron Nanocrystallography, is an Innovative Training Network, Marie Skłodowska-Curie Actions, project funded by EU - #IIT

Joined July 2021

71 Following 78 Followers


Tweets

Tweets & replies

Media


Likes

You Retweeted



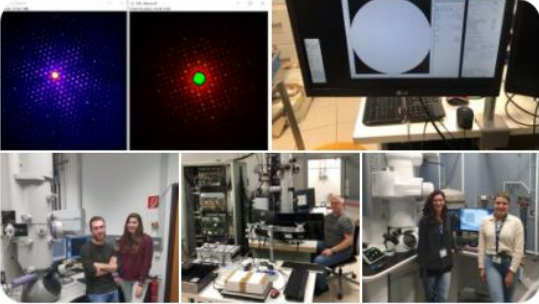
Shao-Liang Zheng @shaoliangzheng · Aug 27

"To teach is to learn twice"- Teaching space-group diagrams to chemistry students through a peer-tutoring approach @HarvardCCB 🤔🤔
scripts.iucr.org/cgi-bin/paper?... @ActaCrystE @IUCr @IUCrTeach
#crystallography #education




scripts.iucr.org
Teaching space-group diagrams to chemistry stud...
`Symmetry and Space Group Tutorial' (by Jerry P. Jasinski and Bruce M. Foxman) provides chemistry

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Trending in Italy

#Bitcoin ₿

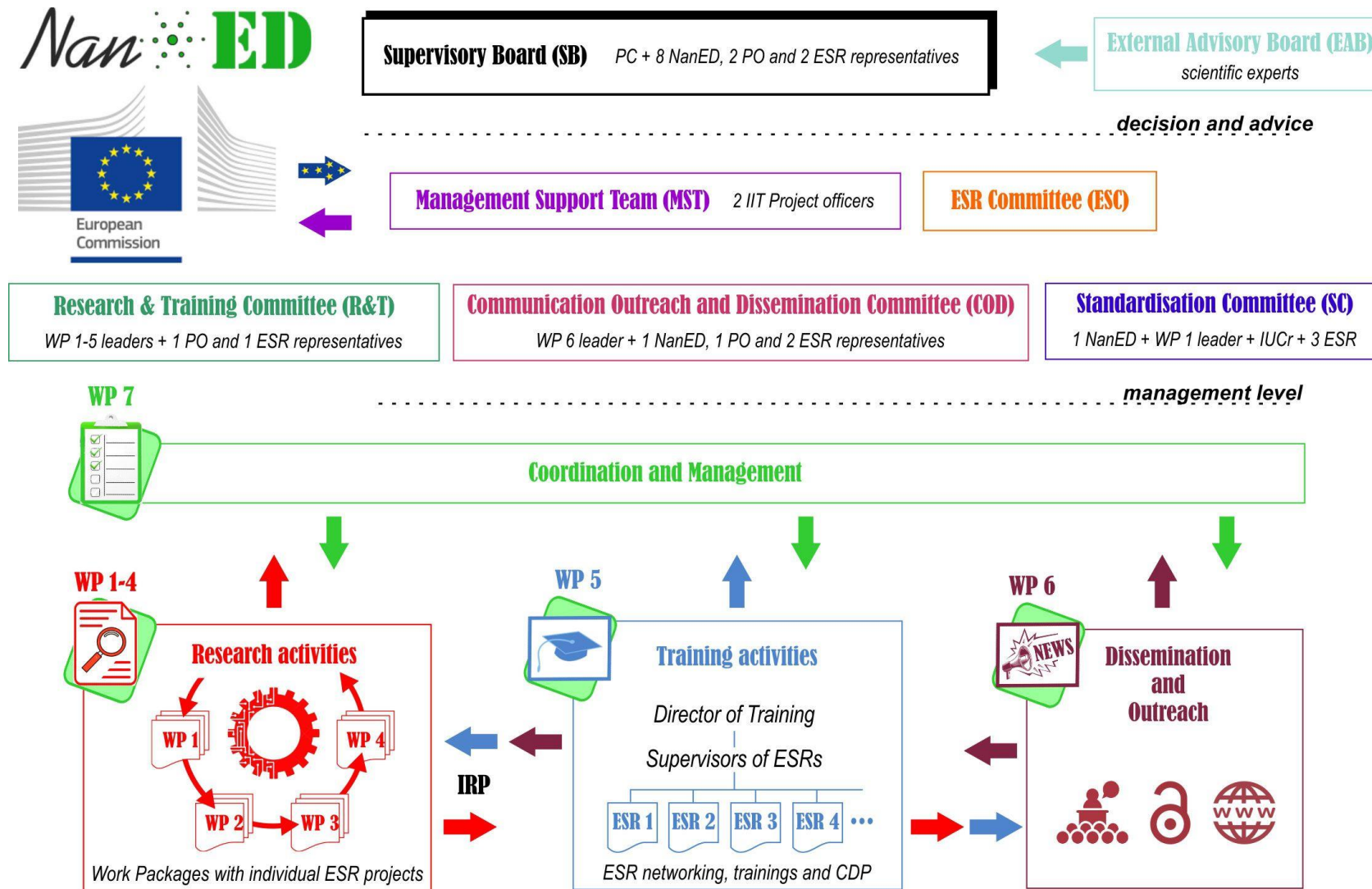
256K Tweets



Naned_project
@NanedP



NanED Governance



NanED: beneficiary of the NanED project

PO: partner organization of the NanED project



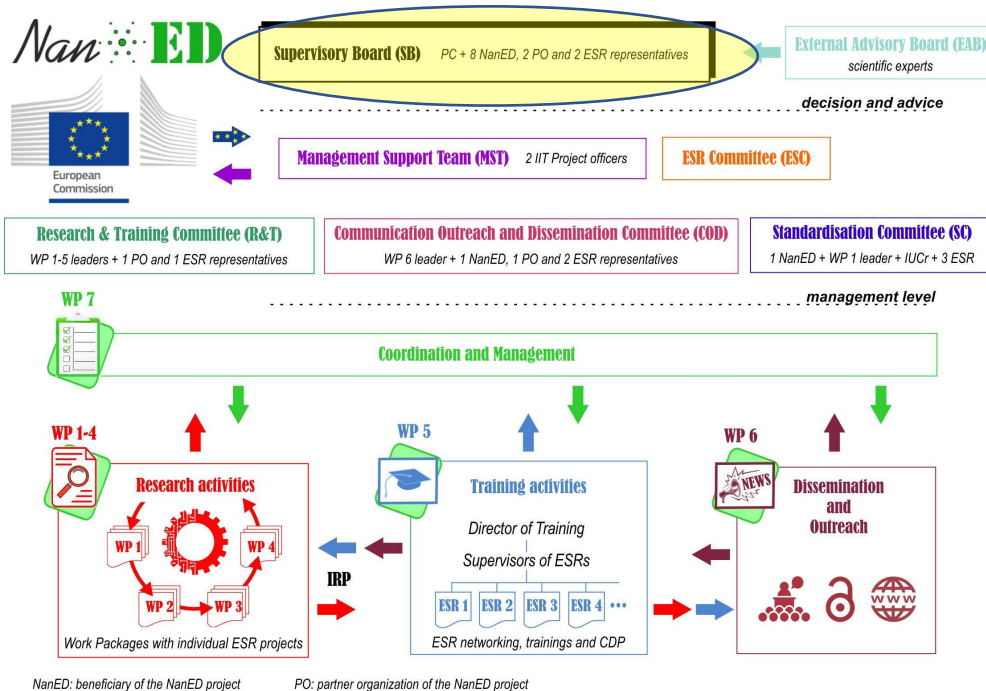
Supervisory Board (SB)

The highest organ in the project and takes all essential decisions.

The SB will be chaired by the project coordinator (PC) and is composed by:

8 Beneficiary + 2 Partners (change every 2 years, have an advisory role) + 2ESR

The SB will be responsible for the strategic decisions and high level monitoring of research and training activities, including CDPs, ESRs recruitment strategy, knowledge transfer, dissemination and outreach.



SB will meet once a year with an increased frequency whenever required.

EAB experts will be invited to the sessions and asked for opinion to improve the supervision capacity of SB and the quality.



External advisory board (EAB)

To reinforce the supervision scheme, a multidisciplinary EAB, composed of reputable experts in NanED's main disciplines will additionally provide guidance on scientific priorities, providing recommendations both during the definition and the monitoring of ESRs' projects and attending the yearly progress meetings.



Sven Hovmöller



Paul Midgley

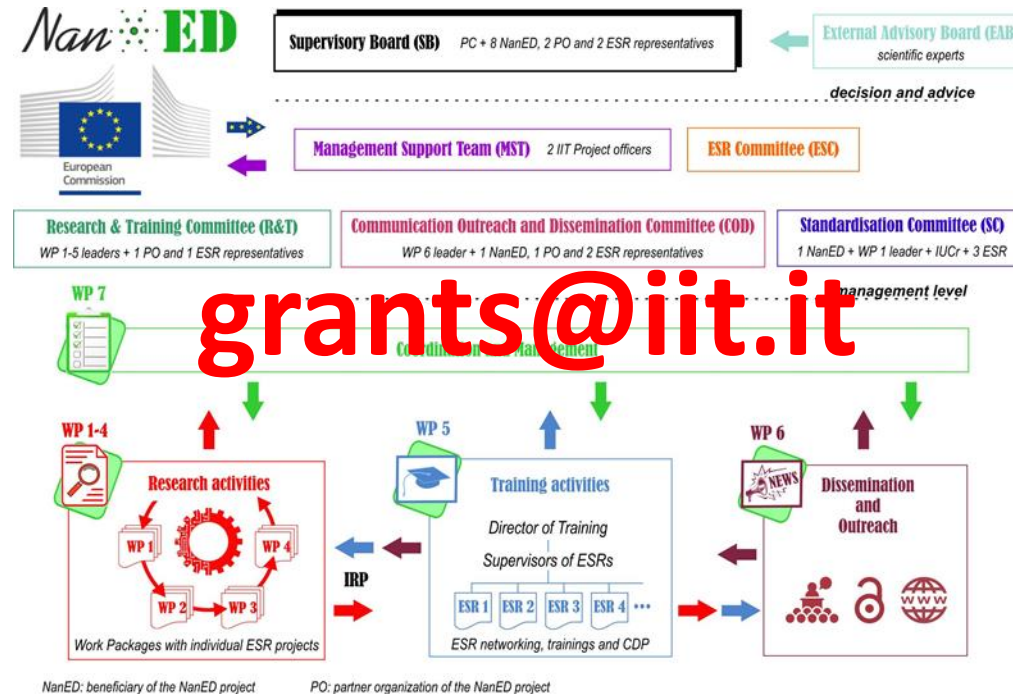


Liberato Manna



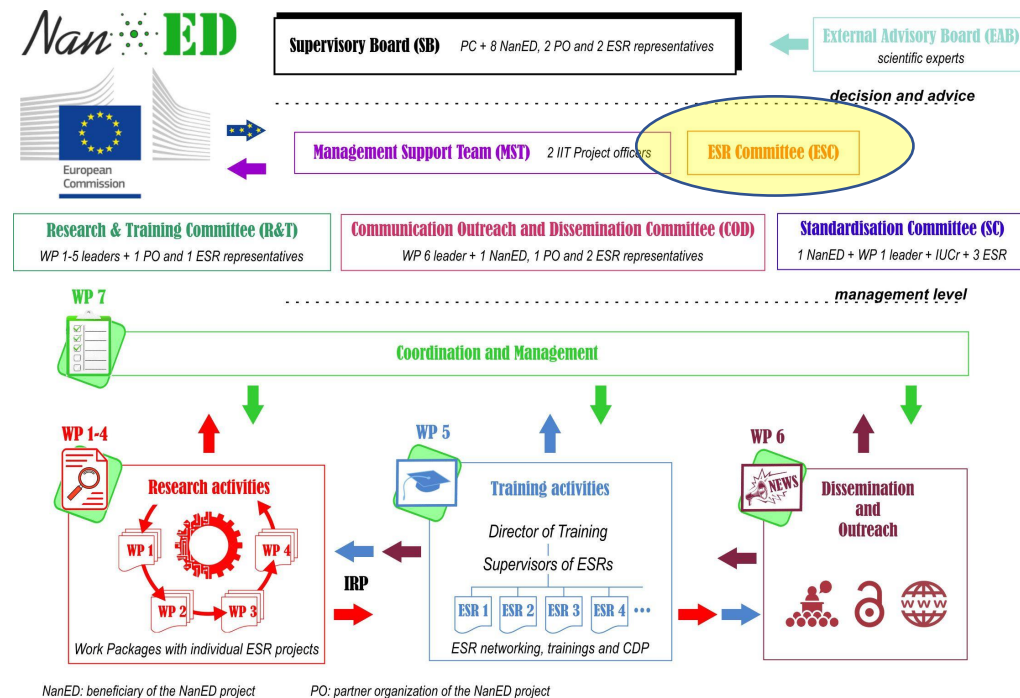
Management Support Team (MST)

Composed by two members of the IIT Projects Office, it will give support to the PC for the administrative and financial management of the project.



ESR Committee (ESC)

All ESRs will be represented in the ESC. **ESC elects the ESR representative in the other committees.** Through them it will report the integration at host institution and general progress of fellows to SB. It will also inform the SB on any issue concerning the implementation of individual research project. The ESC will also foster permanent communication among ESRs and will provide a tool to exchange experiences, clarify questions, identify common demands and potential complaints. The **ESC regularly meet (online/on-site) every 2 months** to discuss scientific issues, contributions to the research and training program and ideas concerning ESRs CDPs.

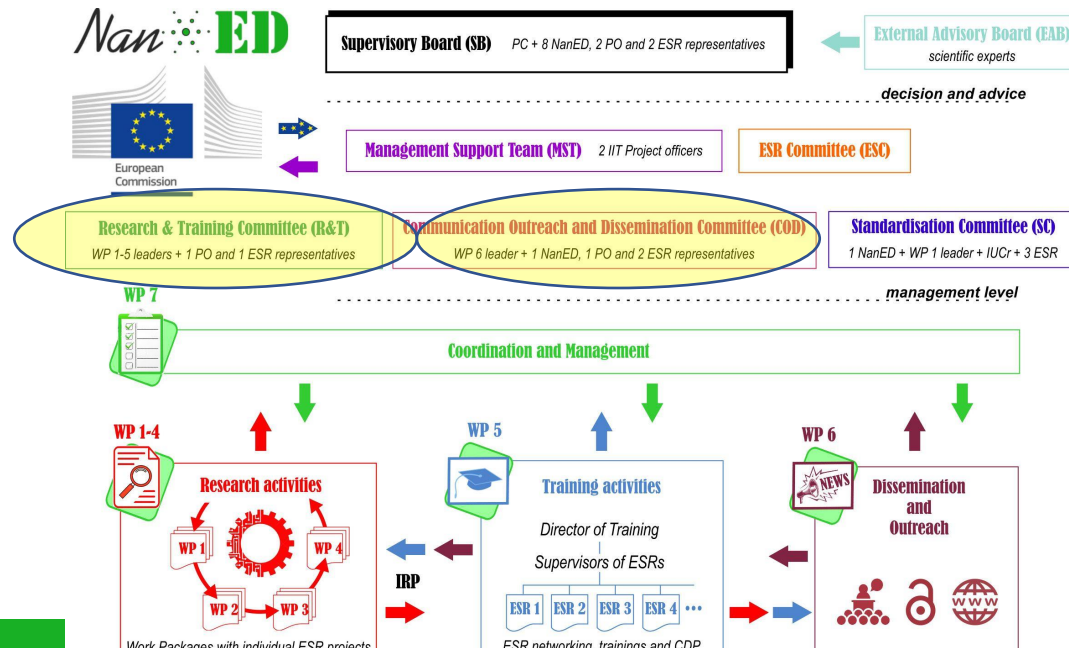


Research & Training Committee (R&T)

Chaired by **Philippe Boullay** (WP5 leader) and participated by the 4 scientific WPs leaders (WP1-4), **by one representative of the partner organizations and one ESR delegated by the ESC**. R&T will supervise the fulfilments of the task objectives related to each work package. It will coordinate, through the WPs leaders, the execution of the deliverables and milestones and be in contact with the SB to report any incident or changes.

Communication Outreach and Dissemination Committee (COD)

Chaired by the **Xiaodong Zou** (WP6 leader) and participated by another beneficiary, **one partner organization and 2 ESR representative**. It will be responsible of scheduling, monitoring and evaluating NanED's communication, outreach and dissemination activities. It will coordinate and monitor the dissemination communication and exploitation plan.

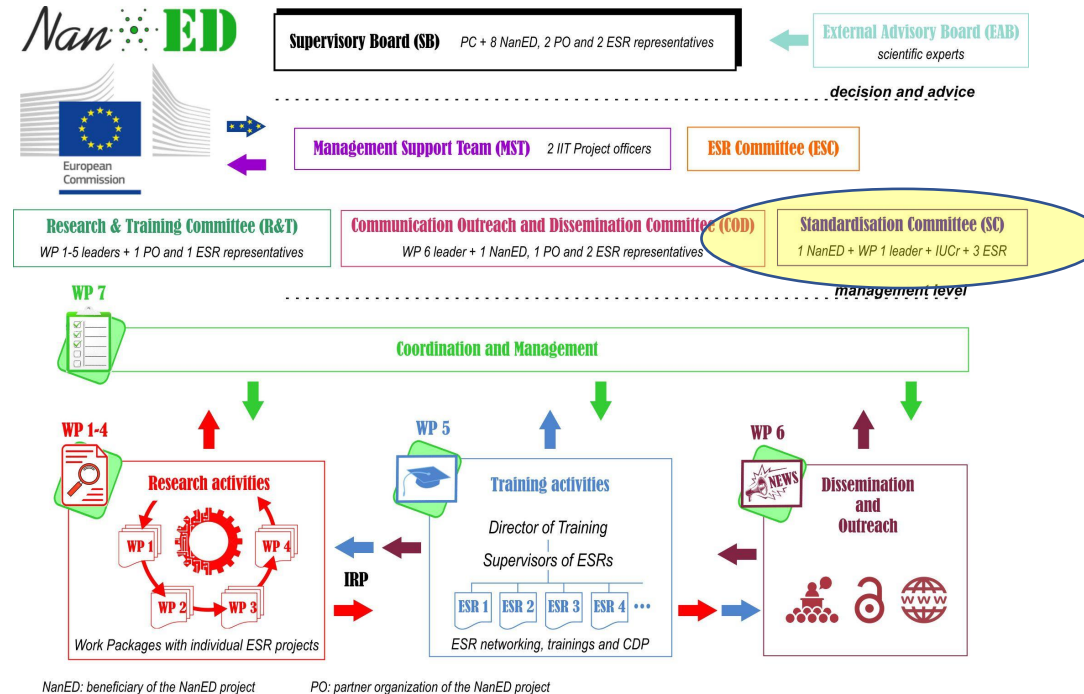


Standardization Committee (SC)

Chaired by one of the beneficiaries (elected during the first SB meeting) and participated by the WP1 leader, by the IUCr scientist in charge and by the **3 ESRs** that will do a secondment at IUCr. It will be the organ responsible for gathering all the information from the beneficiaries necessary for inserting into the cif file format all the specifications for crystal structures solved and refined with 3D ED.

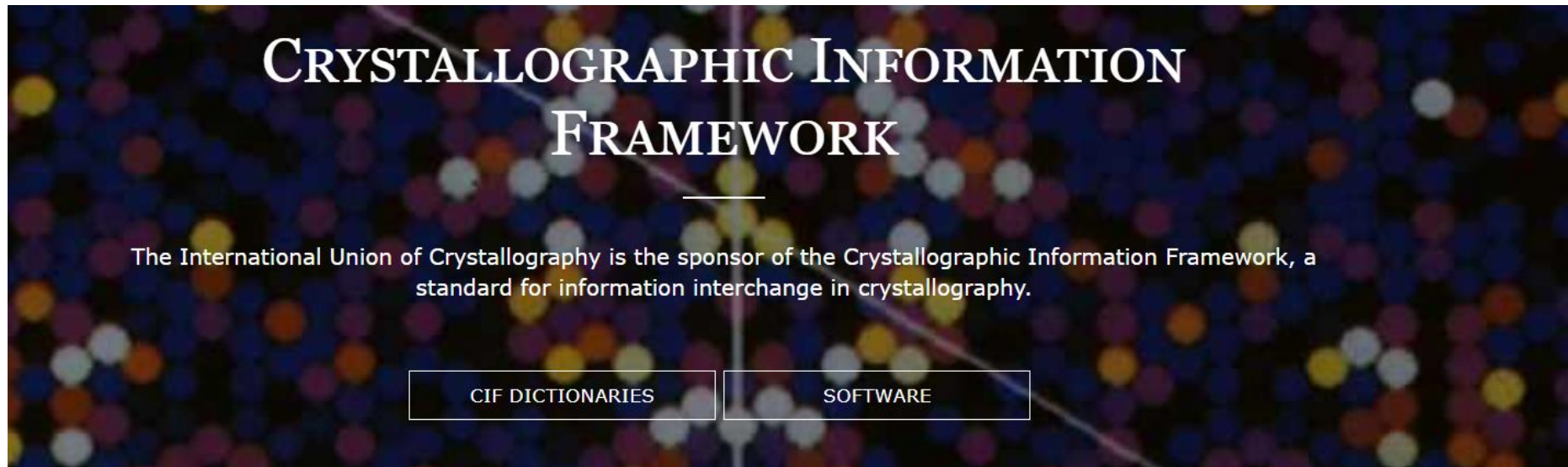


I will schedule a meeting soon!!!!





Standardization Committee (SC)

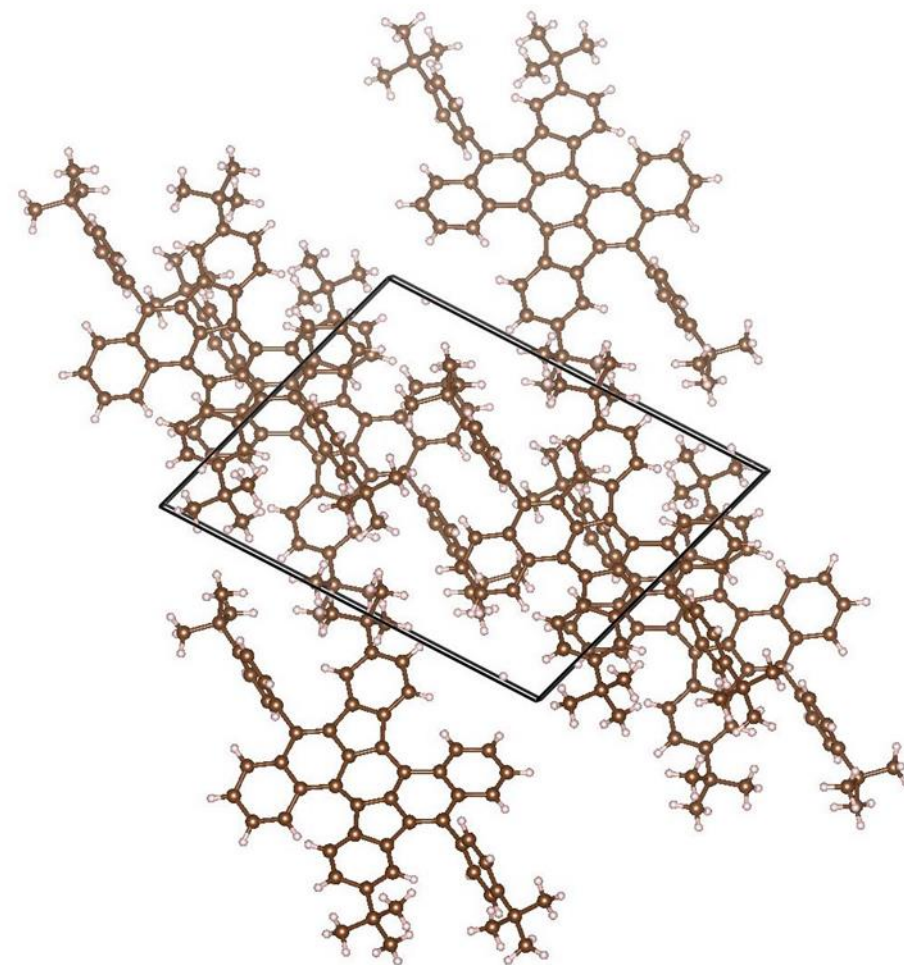


The acronym CIF is used both for the **Crystallographic Information File**, the data exchange standard file format of Hall, Allen & Brown (1991) (see Documentation), and for the Crystallographic Information Framework, a broader system of exchange protocols based on data dictionaries and relational rules expressible in different machine-readable manifestations, including, but not restricted to, Crystallographic Information File and XML.



_cell_length_a	10.720 (6)
_cell_length_b	13.870 (7)
_cell_length_c	18.37 (2)
_cell_angle_alpha	101.39 (3)
_cell_angle_beta	106.35 (2)
_cell_angle_gamma	106.679 (16)
_cell_volume	2393 (3)
_cell_formula_units_Z	2
_cell_measurement_temperature	303 (2)
_cell_measurement_reflns_used	3605
_cell_measurement_theta_min	0.057
_cell_measurement_theta_max	0.960

_exptl_crystal_description	'nanocrystal'
_exptl_crystal_colour	'orange'
_diffrn_ambient_temperature	303 (2)
_diffrn_radiation_wavelength	0.0335
_diffrn_radiation_type	'electron'
_diffrn_source	'120 kV electron microscope'
_diffrn_source_type	'LaB6 gun'
_diffrn_measurement_device	'transmission electron microscope'
_diffrn_measurement_device_type	'Zeiss Libra 120'
_diffrn_detector	'single-electron detector MEDIPIX'
_diffrn_detector_type	'ASI Timepix'
_diffrn_measurement_method	'stepwise precession-assisted 3D electron diffraction'




```

loop_
  _atom_site_label
  _atom_site_type_symbol
  _atom_site_fract_x
  _atom_site_fract_y
  _atom_site_fract_z
  _atom_site_U_iso_or_equiv
  _atom_site_adp_type
  _atom_site_occupancy
  _atom_site_site_symmetry_order
  _atom_site_calc_flag
  _atom_site_refinement_flags_posn
  _atom_site_refinement_flags_adp
  _atom_site_refinement_flags_occupancy
  _atom_site_disorder_assembly
  _atom_site_disorder_group

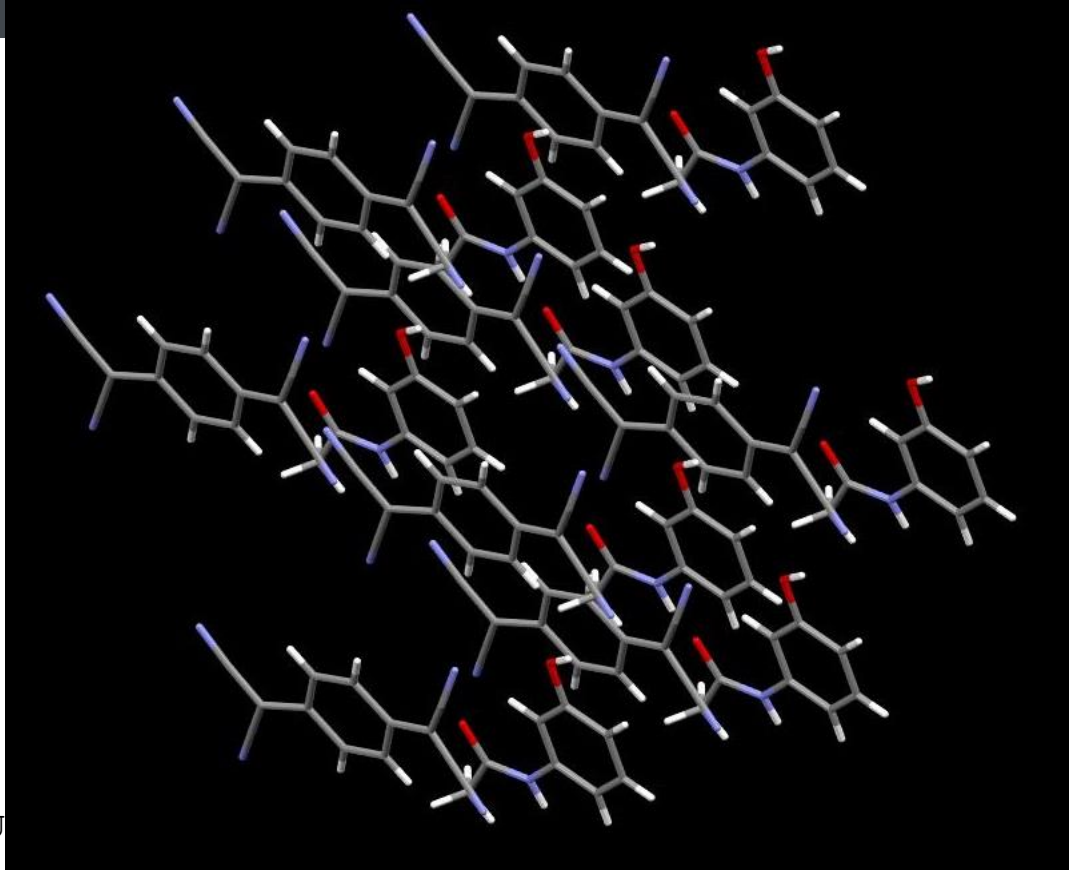
```

```

C1_1 C 0.2413(17) 0.6578(12) 0.9149(8) 0.022(7) Uiso 1 1 d D U . . .
C2_1 C 0.207(2) 0.7435(14) 0.9001(10) 0.036(8) Uiso 1 1 d D U . . .
H2_1 H 0.201049 0.756204 0.851579 0.043 Uiso 1 1 calc R U . . .
C3_1 C 0.182(2) 0.8100(16) 0.9563(10) 0.036(8) Uiso 1 1 d D U . . .
H3_1 H 0.157277 0.865577 0.944219 0.043 Uiso 1 1 calc R U . . .
C4_1 C 0.
C5_1 C 0.
H5_1 H 0.235378 0.700473 1.096593 0.053 Uiso 1 1 calc R U . . .
C6_1 C 0.2485(18) 0.6419(12) 0.9899(8) 0.025(7) Uiso 1 1 d D U . . .
C7_1 C 0.2702(16) 0.5416(12) 0.9887(8) 0.017(7) Uiso 1 1 d D U . . .
C8_1 C 0.2802(15) 0.4867(11) 1.0438(7) 0.019(7) Uiso 1 1 d D U . . .
C9_1 C 0.3101(17) 0.3918(11) 1.0265(8) 0.021(7) Uiso 1 1 d D U . . .

```

3ESR will participate to this committee but all will contribute!!!!



NanED GANTT

	2021	1	2	3	4	5	6	7	8	9	10	2022	11	12	13
		Mar	Apr	May	June	July	Aug	Sep	Oct	Nov	Dec		Jan	Feb	Mar
IIT			D6.1 - D7.1 - D7.2							JIM	D5.2			D8.1 - <u>MS1</u>	
CNRS											D5.1				
FZU							D6.2								
JGU															
SU														D6.3	D7.3
UA															
UBA															
ULM															
Event										JIM					

The project has Deliverables and Milestones and Events



NanED GANTT

	2021	1	2	3	4	5	6	7	8	9	10	2022	11	12	13
		Mar	Apr	May	June	July	Aug	Sep	Oct	Nov	Dec		Jan	Feb	Mar
IIT			D6.1 - D7.1 - D7.2							JIM	D5.2			D8.1 - <u>MS1</u>	
CNRS											D5.1				
FZU							D6.2								
JGU															
SU														D6.3	D7.3
UA															
UBA															
ULM															
Event										JIM					

D7.1	2	IIT	Consortium Agreement		
D7.2	2	IIT	Supervisory board of the network		
D6.1	2	IIT	Web site + logo		
D6.2	6	FZU	Data managment plan I		
D5.1	10	CNRS	CDP for each ESR		
D5.2	10	IIT	Joint initial Meeting Report		

← Done

← Done

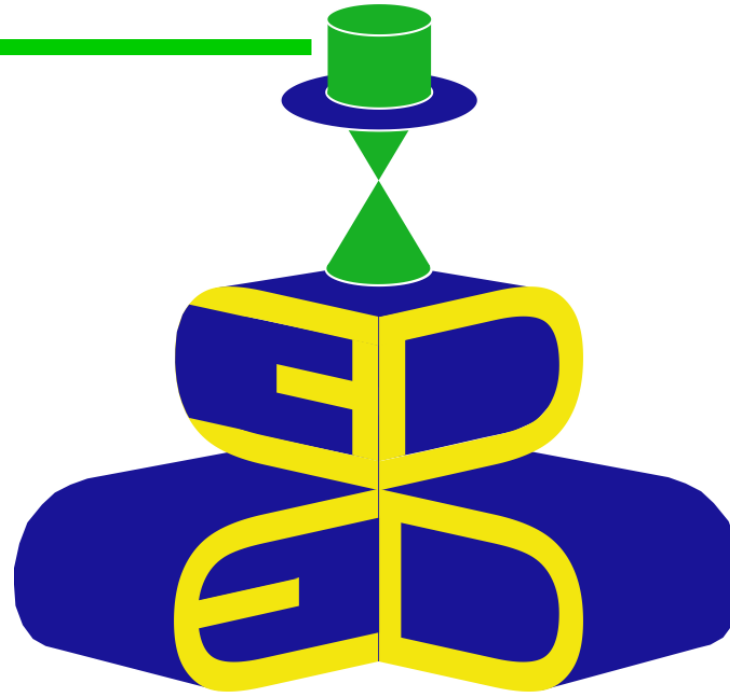
← To be postponed



NanED LOGO

Green
the electron colour

3D ED
symbol



The colours of
the EU flag

Nan • • • **ED**

© by Philippe Boullay



NanED GANTT

	2021	1	2	3	4	5	6	7	8	9	10	2022	11	12	13
		Mar	Apr	May	June	July	Aug	Sep	Oct	Nov	Dec		Jan	Feb	Mar
IIT			D6.1 - D7.1 - D7.2							JIM	D5.2			D8.1 - <u>MS1</u>	
CNRS											D5.1				
FZU							D6.2								
JGU															
SU														D6.3	D7.3
UA															
UBA															
ULM															
Event										JIM					

D7.1	2	IIT	Consortium Agreement		
D7.2	2	IIT	Supervisory board of the network		
D6.1	2	IIT	Web site + logo		
D6.2	6	FZU	Data management plan I		
D5.1	10	CNRS	CDP for each ESR		
D5.2	10	IIT	Joint initial Meeting Report		

D6.3	12	SU	dissemination comm. Exploit. Plan		
D7.3	13	IIT	Progress report		
D8.1	12	IIT	Ethics requirements		
<u>MS1</u>	12	IIT	Recruitment completed		



NanED GANTT

	2022	11	12	13	14	15	16	17	18	19	20	21	22	2023	23	24
		Jan	Feb	Mar	Apr	May	June	July	Aug	Sep	Oct	Nov	Dec		Jan	Feb
IIT			D8.1 - <u>MS1</u>			<u>MS2</u>			D1.1		D1.2					D1.4
CNRS																
FZU						WS1	D5.3									D3.1 - D6.4
JGU													WS2		D5.4	
SU			D6.3	D7.3												D1.3 - D2.1 <u>MS3</u>
UA																
UBA																
ULM																
Event						WS1							WS2			

D6.3	12	SU	dissemination comm. Exploit. Plan	<u>MS2</u>	15	IIT	Mid term meeting
------	----	----	-----------------------------------	------------	----	-----	------------------

D7.3	13	IIT	Progress report
------	----	-----	-----------------

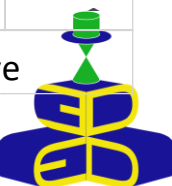
D8.1	12	IIT	Ethics requirements
------	----	-----	---------------------

<u>MS1</u>	12	IIT	Recruitment completed
------------	----	-----	-----------------------



D5.3	16	FZU	Report on WS1
------	----	-----	---------------

D1.1	18	IIT	Round Robin			
D1.2	20	IIT	Protocols 3D ED on beam sensitive			



D1.1

Round Robin of 3D ED on a test sample among all labs (M18)

It was a specific request of the project officer to have a scientific deliverable at the early stage

It is made for the ESR to practice with 3D ED

We need to decide the test sample and to make it available to the consortium

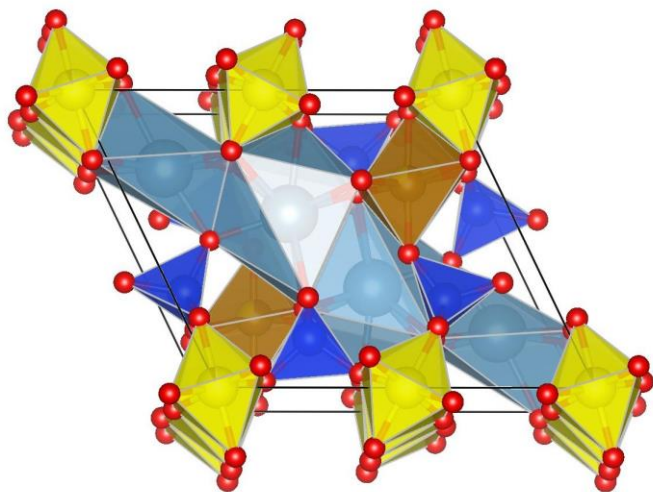
It can be an ideal case for a joint publication of the consortium and the first time the same sample will be analyzed by different labs, different TEMS different data collection types, different detectors.

**Start to think about the
material**



D1.1

Round Robin of 3D ED on a test sample among all labs (M18)

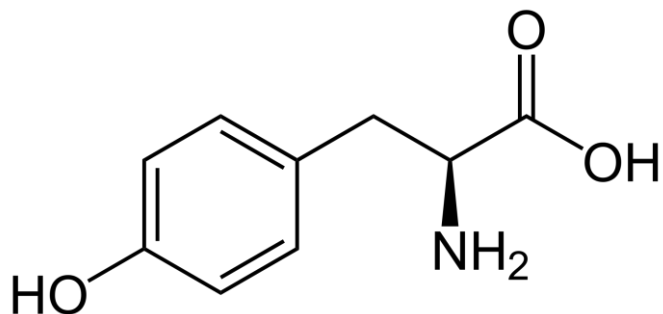


Epidote: $\text{Ca}_2\text{Al}_2(\text{Fe}^{3+};\text{Al})(\text{SiO}_4)(\text{Si}_2\text{O}_7)\text{O}(\text{OH})$

Monoclinic $P2_1/m$

$a=8.9$ $b=5.6$ $c=10.2$ $\beta=115^\circ$

21 atoms in the asymmetric unit + 1 H



L-Tyrosine: $\text{C}_9\text{H}_{11}\text{NO}_3$

Orthorhombic $P2_12_12_1$

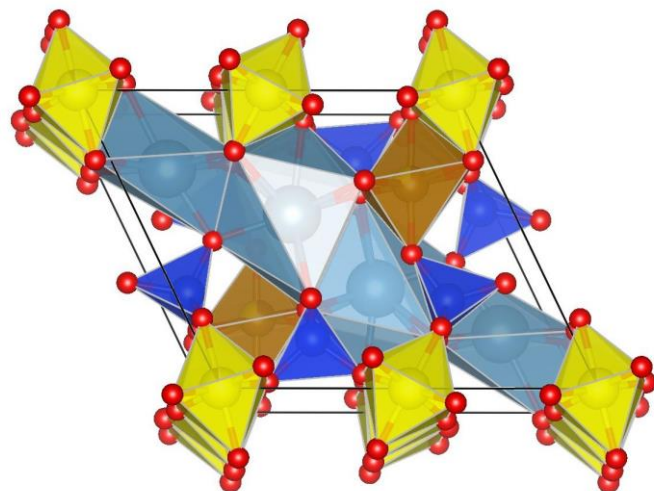
$a=6.9$ $b=21.2$ $c=5.8$

13 atoms in the asymmetric unit without H



D1.1

Round Robin of 3D ED on a test sample among all labs (M18)

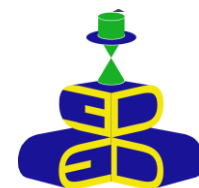
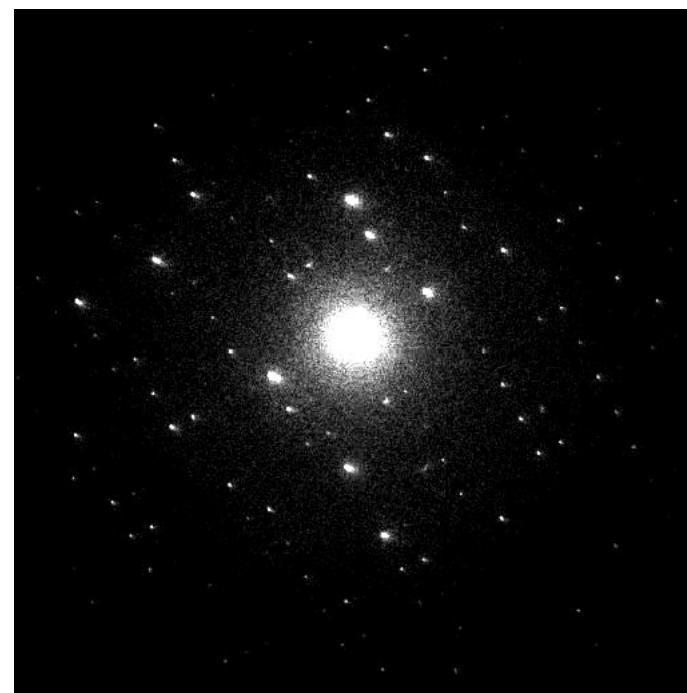
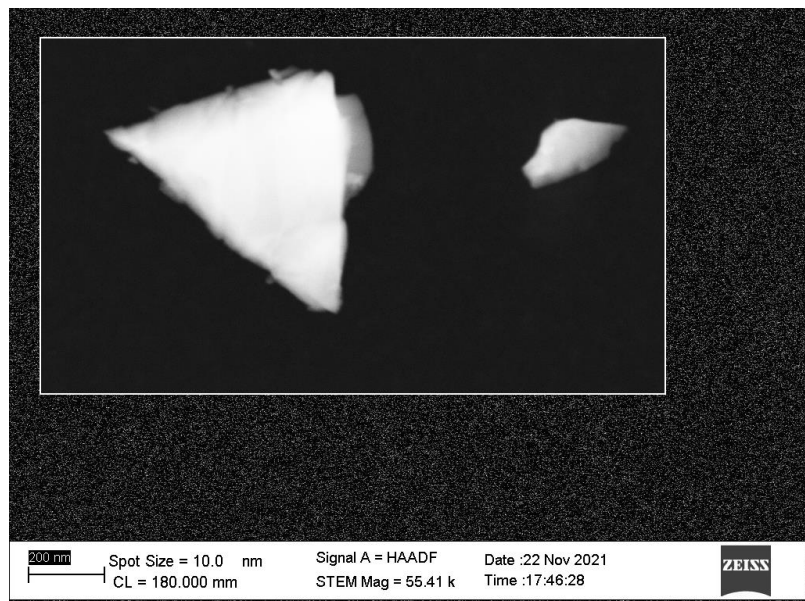


Epidote: $\text{Ca}_2\text{Al}_2(\text{Fe}^{3+};\text{Al})(\text{SiO}_4)(\text{Si}_2\text{O}_7)\text{O}(\text{OH})$

Monoclinic $P2_1/m$

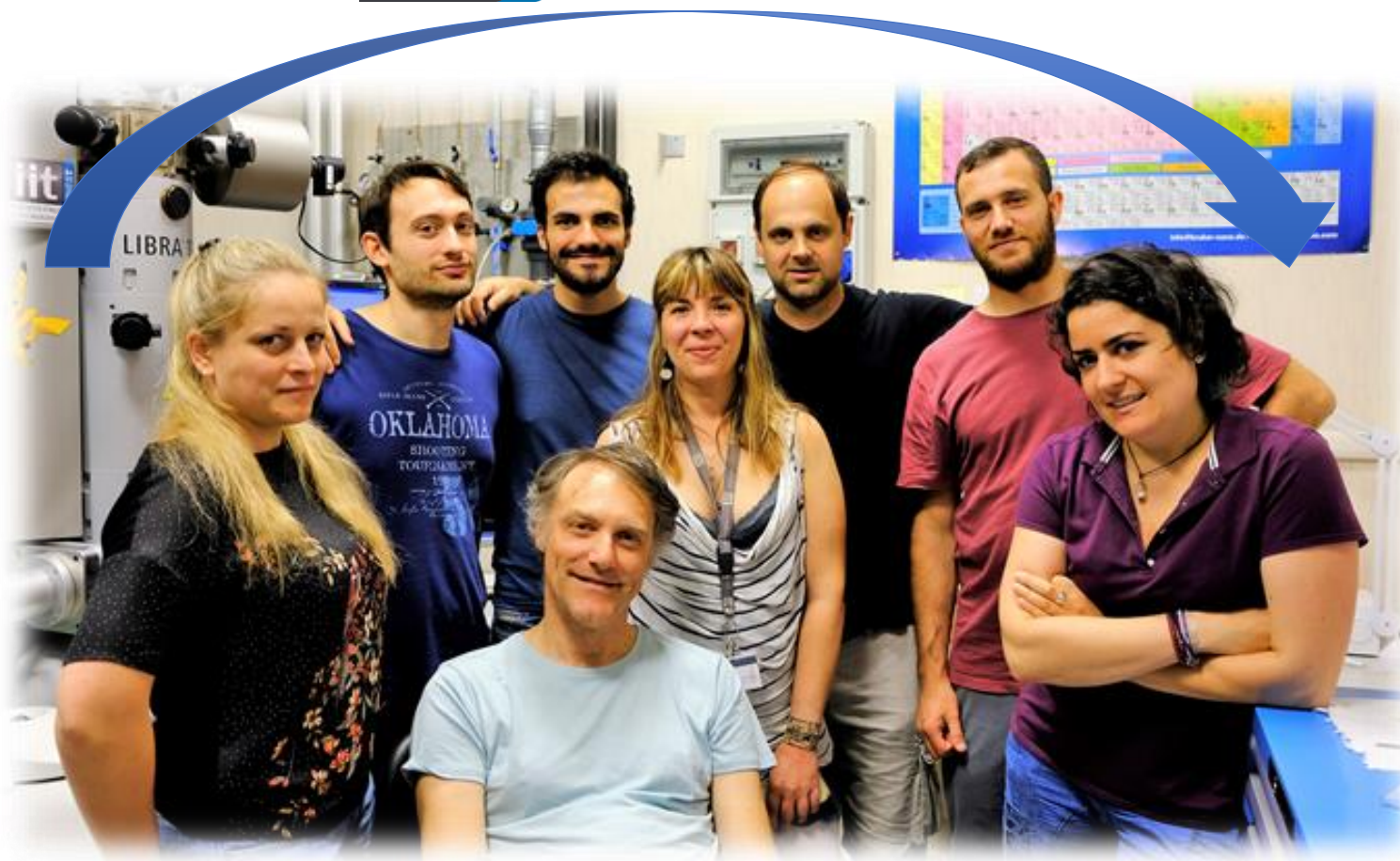
$a=8.9$ $b=5.6$ $c=10.2$ $\beta=115^\circ$

21 atoms in the asymmetric unit + 1 H





Paola Parlanti



Giovanna Molinari (Unipi)

Following the arrow: Iryna Andrusenko, Francesco Papi, Andrea Griesi, Valentina Cappello, Enrico Mugnaioli, Fabrizio Campanale, Arianna Lanza

Not in the picture Elena Husanu, Andrea Sala, Danilo Marchetti Daniele Sonaglioni



Thank you

