



H2020-MSCA ITN  
Grant n. 956099



*Nan*ED



# WP6 - Dissemination and Communication

Hongyi Xu – Stockholm University

# Dissemination and Communication



*Nan* • • • **ED**

## The Nan Ed Project

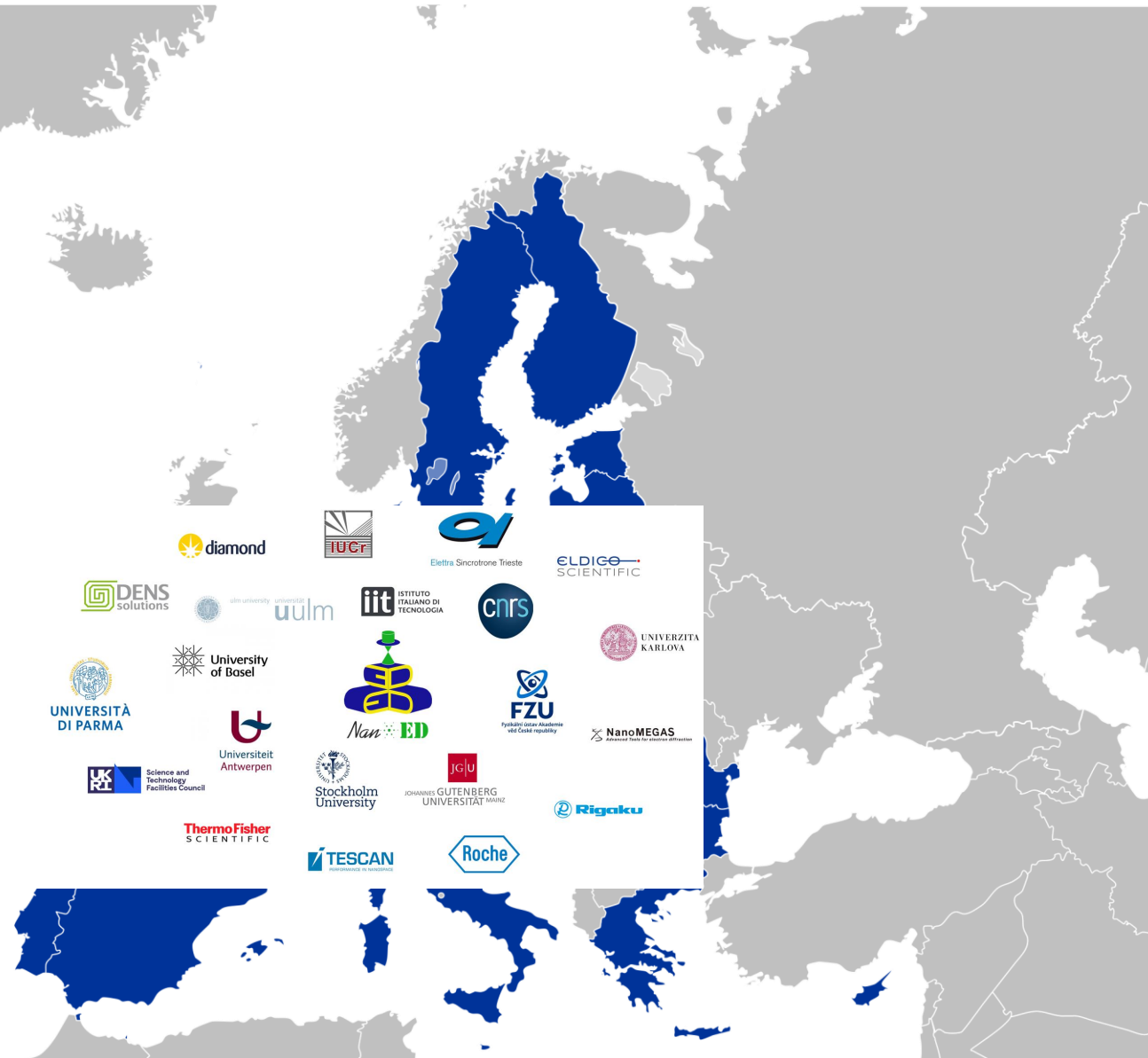
The Nan ED Project - Electron Nanocrystallography, is an Innovative Training Network, Marie Skłodowska-Curie Actions, project funded by EU (grant agreement n. 956099) aimed to train a new generation of electron crystallographers thereby paving the way for future development and establishment of the method more broadly in the academic community and within the industry.



# Dissemination and Communication



# Dissemination and Communication



- To train a new generation of electron crystallographers
- Future development and establishment of electron crystallography
- Benefit to the society
  - Crystallography
  - Chemistry and Biology
  - Smart materials
    - Energy
    - Resources
    - Renewable
  - New drugs
- EU and World



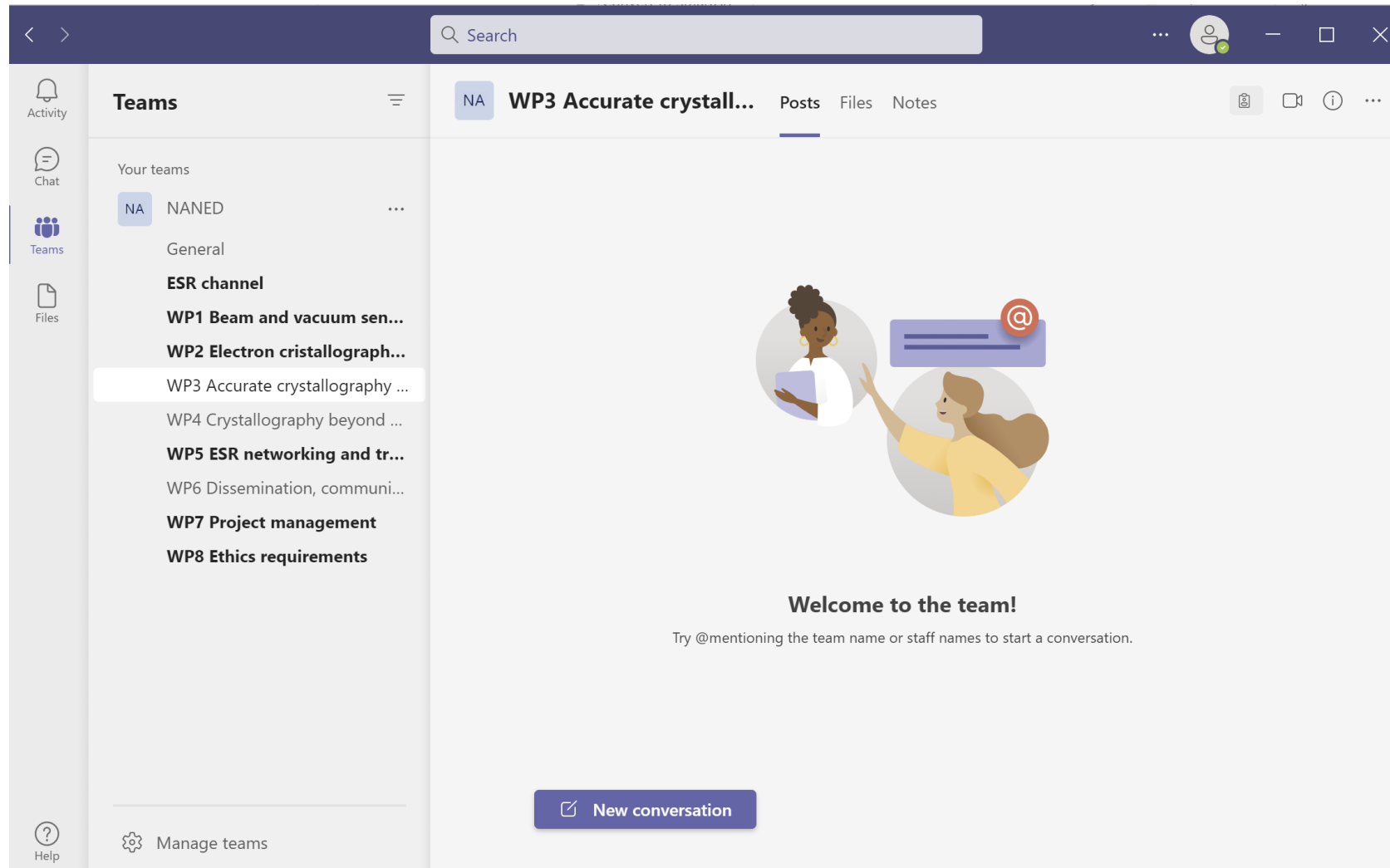
# Host Group

- PhD Training:
  - Individual meeting with main and co-supervisors (i.e. twice per month)
  - Group Meetings (i.e. 3 formal presentations per year)
  - Secondment – Establishing communications, mentorship
- Integration of the student to the research group
- Open communications:
  - Change of supervisors
    - ESR 7 -> SU
  - Seeking assistance



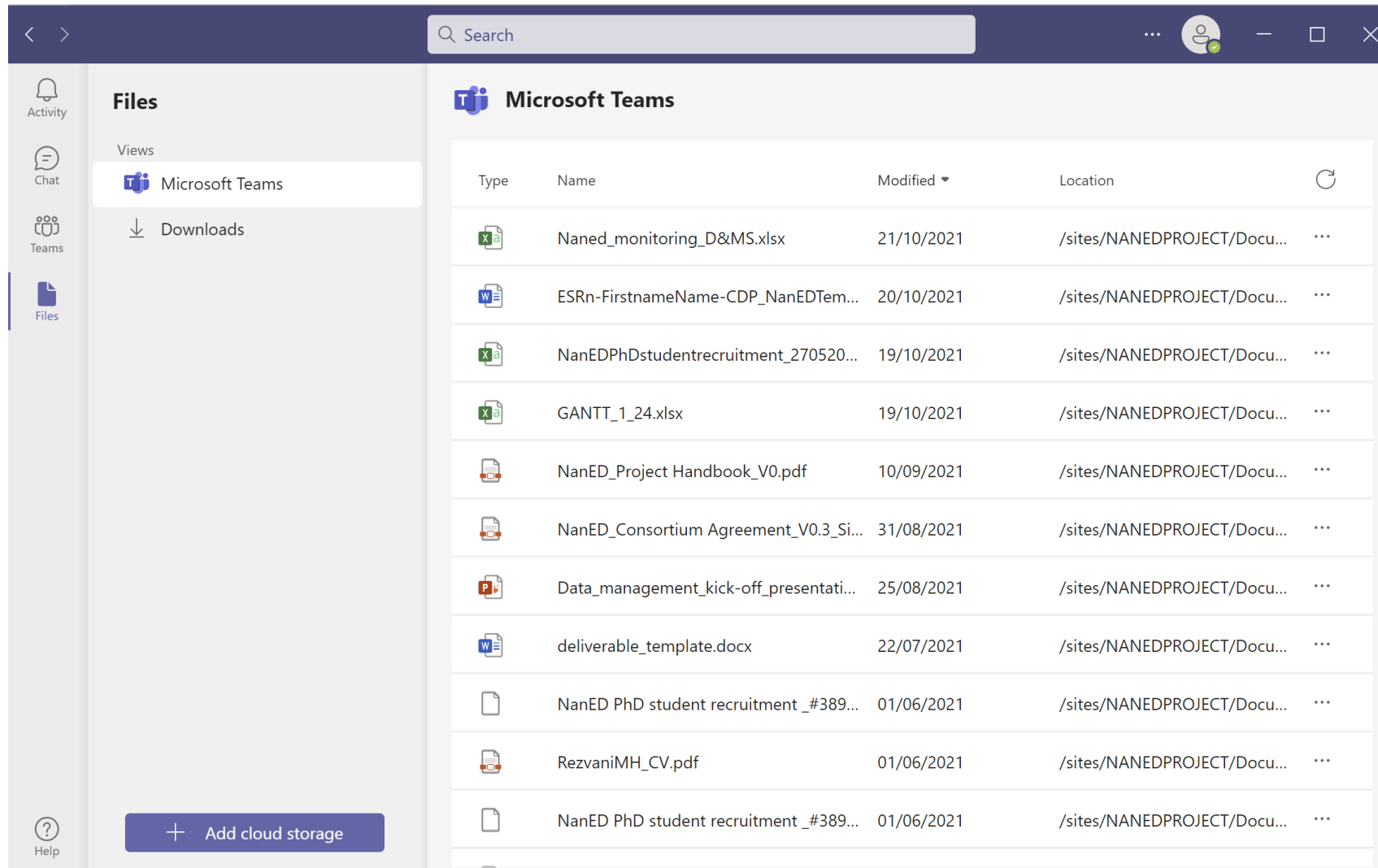
# Platform for Communication among ESRs

- Promote active discussions and communications
- Microsoft teams



# Platform for Communication among ESRs

- Promote active discussions and communications
- Microsoft teams



The screenshot displays the Microsoft Teams application interface. On the left, a sidebar contains navigation icons for Activity, Chat, Teams, and Files. The main area is titled 'Files' and shows a list of documents. The 'Views' section is set to 'Microsoft Teams'. Below this, there is a 'Downloads' section. The file list table includes columns for Type, Name, Modified, and Location. The files listed are:

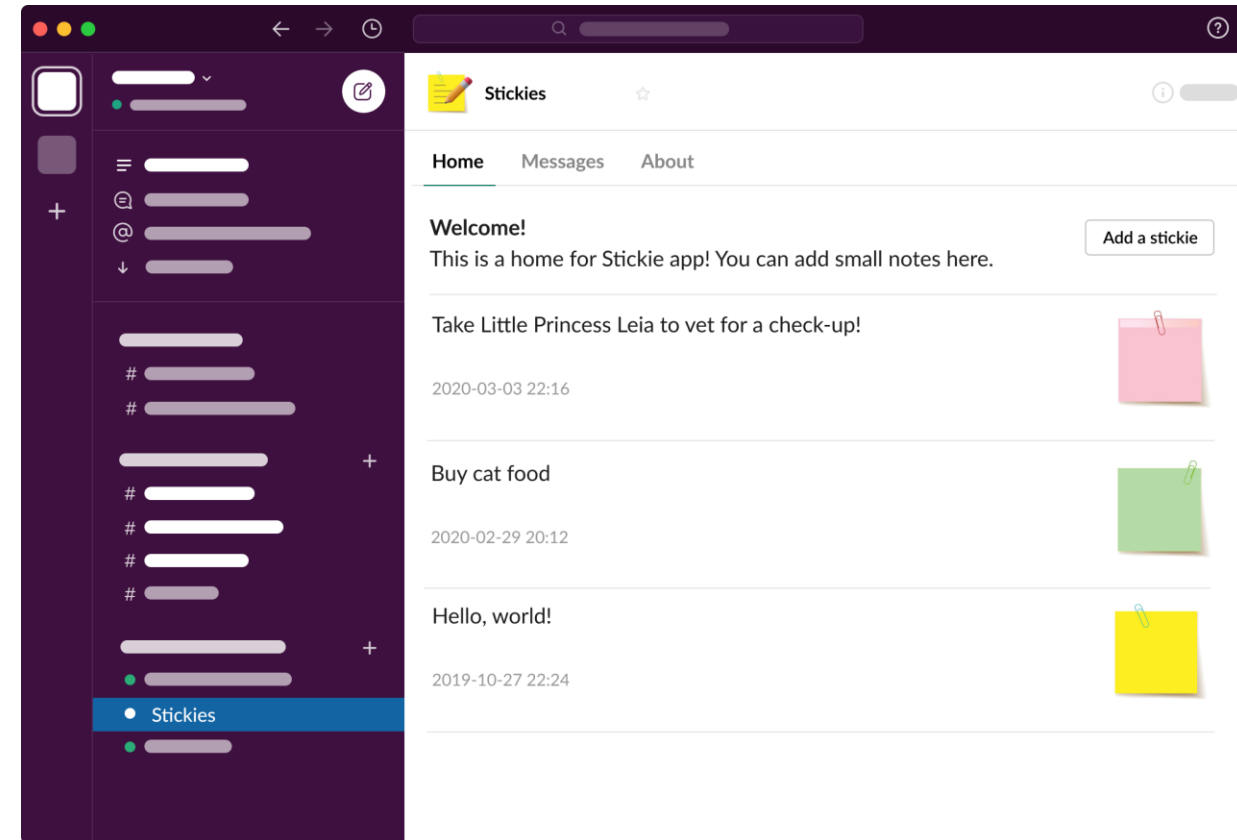
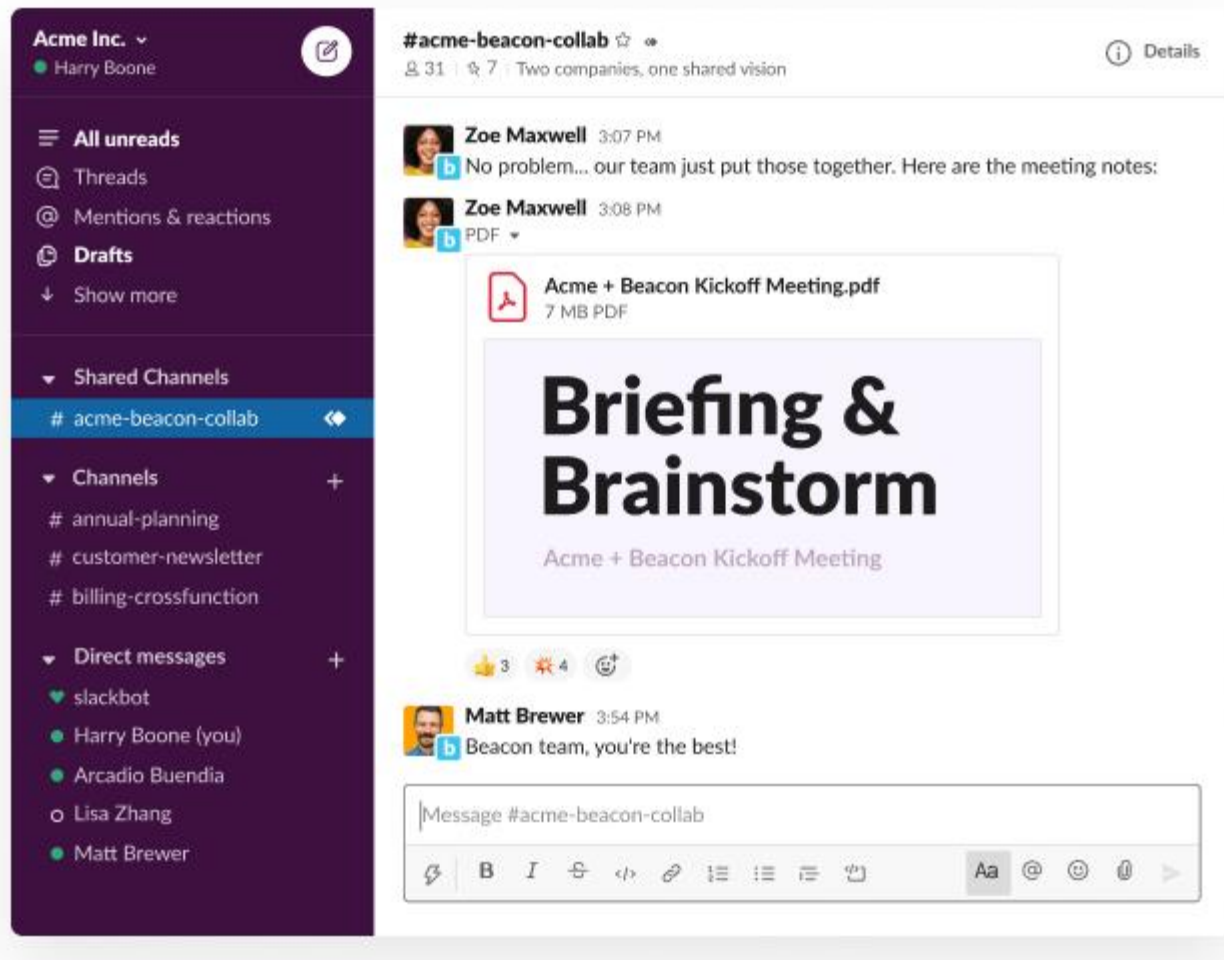
Type	Name	Modified	Location
Excel	Naned_monitoring_D&MS.xlsx	21/10/2021	/sites/NANEDPROJECT/Docu...
Word	ESRn-FirstnameName-CDP_NanEDTem...	20/10/2021	/sites/NANEDPROJECT/Docu...
Excel	NanEDPhDstudentrecruitment_270520...	19/10/2021	/sites/NANEDPROJECT/Docu...
Excel	GANTT_1_24.xlsx	19/10/2021	/sites/NANEDPROJECT/Docu...
PDF	NanED_Project Handbook_V0.pdf	10/09/2021	/sites/NANEDPROJECT/Docu...
PDF	NanED_Consortium Agreement_V0.3_Si...	31/08/2021	/sites/NANEDPROJECT/Docu...
PowerPoint	Data_management_kick-off_presentati...	25/08/2021	/sites/NANEDPROJECT/Docu...
Word	deliverable_template.docx	22/07/2021	/sites/NANEDPROJECT/Docu...
Document	NanED PhD student recruitment _#389...	01/06/2021	/sites/NANEDPROJECT/Docu...
PDF	RezvaniMH_CV.pdf	01/06/2021	/sites/NANEDPROJECT/Docu...
Document	NanED PhD student recruitment _#389...	01/06/2021	/sites/NANEDPROJECT/Docu...

At the bottom of the sidebar, there is a 'Help' icon and a button labeled '+ Add cloud storage'.



# Platform for Communication among ESRs

- Promote active discussions and communications
- Slack





# Platform for Communication with Partners

- Sharing of new results/new possibilities
- New wishes to/from the partners
- Suitable samples from partners
- Demonstrations, test of new equipments
- Why of communication:
  - Direct communications
  - Group communication via Microsoft teams



# Dissemination and Communication Tasks

- **Dissemination**

- Project Website
- Journal Publications
- Conference Attendance
- Data Repository
- Workshop at Conferences
- Final Conference

We will establish working groups

2 ESRs will join the dissemination and communication committee

- **Communication**

- Communication Material
- Social Media
- Blog
- Newsletter
- Societal Engagement Events
- European Nights of Researchers



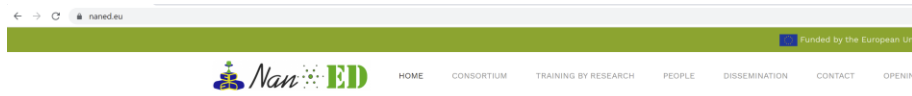
# Project Website

- **Information:**

- Research Results
- Press Releases
- Training Materials
- News and Blog
- Other public material
- Links to social media
- Workshops and schools

## News

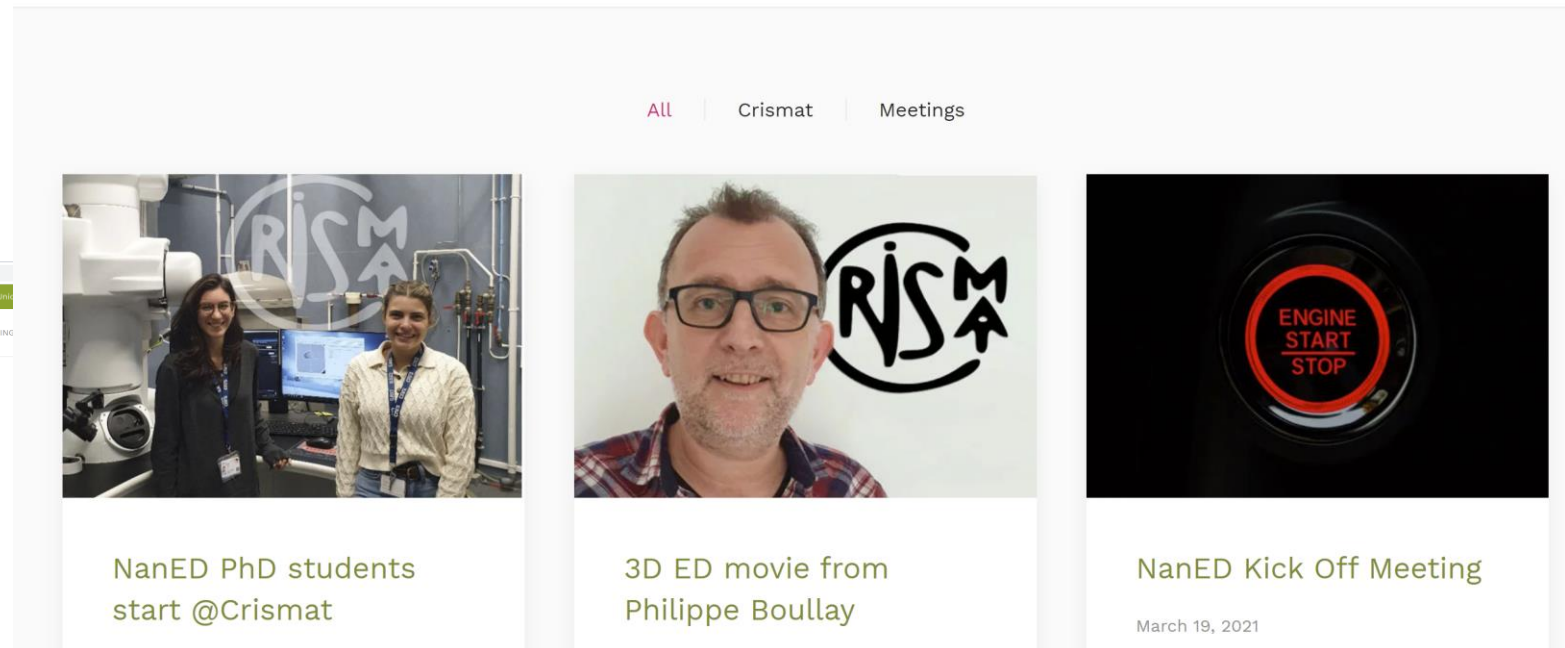
Welcome to NanED news page where you can find out about the Nan ED project's progress as well as events, and related news at a national and international level.



NanED

The Nan Ed Project

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# Project Website

- People:
  - ESRs, Researchers and Supervisors



## PhD Students



Laura Gemmrich Hernandez  
JGU



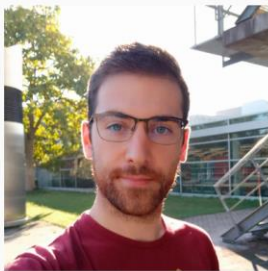
Amatassalam Ben Meriem  
UB



Erica Cordero Oyonarte  
CNRS



Sara Passuti  
CNRS



Marco Santucci  
JGU



Lei Wang  
SU

## Supervisors

All Project Coordinator WP Leader



Mauro Gemmi  
Project Coordinator and WP1/7  
leader



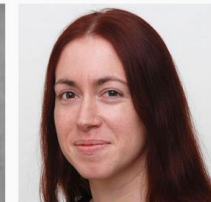
Jan Pieter Abrahams  
WP2 leader



Philippe Boullay  
WP5 leader



Tatiana Gorelik



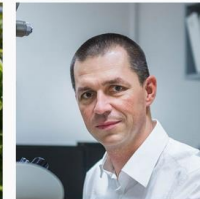
Joke Hadermann



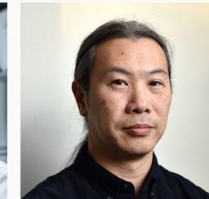
Ute Kaiser



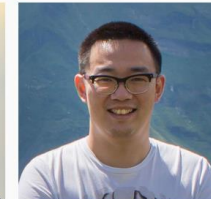
Ute Kolb



Lukas Palatinus  
WP3 leader



Cheuk-Wai Tai



Hongyi Xu



Xiaodong Zou  
WP6 leader





# Project Website

## Linking up ESRs, researchers and stakeholders

- Introducing research demands and ideas

### Lei Wang

Lei Wang got his Bachelor degree in Chemical Technology at Zhengzhou University in 2018. Then he got his Master degree in Environmental Engineering at Zhengzhou University and joint education by Dalian Institute of Chemical Physics in 2021. The aim of his Master project was to investigate the host-guest interactions between molecular sieve frameworks and organic structure-directing agents (OSDAs), which would direct the synthesis of desired molecular sieves. During his study, he learned the knowledge of crystallography in both powder X-ray diffraction (PXRD) and electron diffraction (ED).

He continued his study of electron crystallography at Stockholm University by applying to the European NanED project. He is now working on the project and developing electron diffraction methods used for protein-ligand interactions at nanoscale. He is expected to solve protein structures with different ligands and enable the method in structure-based drug discovery.

🎓 PhD Project 10: **Development and application of electron crystallography methods for studying protein-ligand interactions.**

👤 Supervisor: **Hongyi Xu**

🏛️ Hosting Institution: **Stockholm University**



Research Theme 10

## Development and application of electron crystallography methods for studying protein-ligand interactions

We will develop electron diffraction based methods for studying protein-ligand interactions in order to achieve structure-based drug discovery.

### Objectives

Conduct a proof of principle study on resolving protein-ligand interactions by using 3D electron diffraction based methods. Develop protocols on sample handling, cryo-EM specimen preparation, data collection and processing, and structure refinement for studying protein-ligand interactions. Develop new software and hardware to improve throughput and reliability of 3D electron crystallography methods in order to realize fragment-based lead screening.

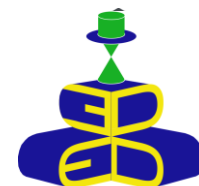
### Expected results

Resolving a test case showing that 3D electron diffraction can be used for studying protein-ligand interactions. Solve a number of protein structures bond with different ligands. A dedicated specimen preparation method for handling protein crystals. The ability to perform fragment-based lead discovery.

- Supervisor  
Dr. Hongji Xu
- Hosting Institution
  - **Stockholms Universitet**
- Planned secondments
  - **UBA**: 3D ED ab-initio phasing on proteins Supervisor: JP. Abrahams
  - **FZU**: Dynamical refinement on organics Supervisor: P. Brázda
  - **Astrazeneca**: Protein ligand interaction Supervisor: H. Käck
  - **eBIC**: Single particle cryoEM Supervisor: P. Zhang
  - **Thermo Fisher**: State of art of cryo TEM

## Intranet for sharing documents

- Password protected
- Each ESR will have a directory: CV; **Career Development Plan**; Publications; Progress reports; Training



# Journal Publication

## Published in High Impact Journals:

- *Nature* Series
- *Science* Series
- *CELL* Press
- ACS journals: such as *JACS* and *ACS Central Science*
- Wiley journals: such as *Angewandte Chemie*
- IUCr journals: *IUCrJ*, *ACTA* series and *Journal of Applied Crystallography*


## Local host requirements

- Number of first authored paper for PhD dissertation
- Open-access policy




# Journal Publication

New Section on Electron Crystallography will be launched in 2022, Main editor: Xiaodong Zou



home archive editors for authors for readers submit open access



**Editorial board**  
ISSN: 2052-2525

**Current issue | Archive**

**IUCrJ** is a fully open-access peer-reviewed journal from the International Union of Crystallography (IUCr).

The journal publishes high-profile articles on all aspects of the sciences and technologies supported by the IUCr *via* its commissions, including emerging fields where structural results underpin the science reported in the article. Our aim is to make **IUCrJ** the natural home for high-quality structural science results. Chemists, biologists, physicists and material scientists are actively encouraged to report their structural studies in **IUCrJ**.

**IUCrJ** covers six broad areas:

- biology and medicine
- chemistry and crystal engineering
- cryoEM
- materials and computation
- neutron and synchrotron science and technology
- physics and free electron laser science and technology

The journal was launched in 2014 to commemorate the International Year of Crystallography.

**More about the journal**

**Journal news**

**Rapid publication of SARS-CoV-2/COVID-19 research in IUCr Journals**

**Submit now at journals.iucr.org/COVID-19**

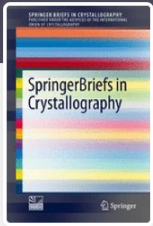
**Why choose IUCrJ?**

- High profile, high impact
- Fast publication, excellent technical editing
- Unlimited readership, fully open access



# Journal Publication

## Springer brief on 3D Electron Diffraction



Book series

### SpringerBriefs in Crystallography

 [Editorial board](#)

## About this book series

SpringerBriefs in Crystallography, published under the auspices of the International Union of Crystallography, aims at presenting highly relevant, concise monographs with an intermediate scope between a topical review and a full monograph. Areas of interest include chemical crystallography, crystal engineering, crystallography of materials (ceramics, metals, organometallics, functional materials), instrumentation, mathematical crystallography, mineralogical crystallography, physical properties of crystals, structural biology and related fields.

SpringerBriefs present succinct summaries of cutting-edge research and practical applications covering a range of content from professional to academic and featuring compact volumes of 50 to 125 pages.

- Under the auspices of IUCr
- Up to 100 pages
- Solo or team work?
- More details to be discussed





# Conference Attendance

## Crystallography conferences:

- IUCr Congress
- European crystallography meeting (**ECM**)
- Crystallography meeting of your home continent



26TH CONGRESS AND  
GENERAL ASSEMBLY OF THE  
INTERNATIONAL UNION OF  
**CRYSTALLOGRAPHY**

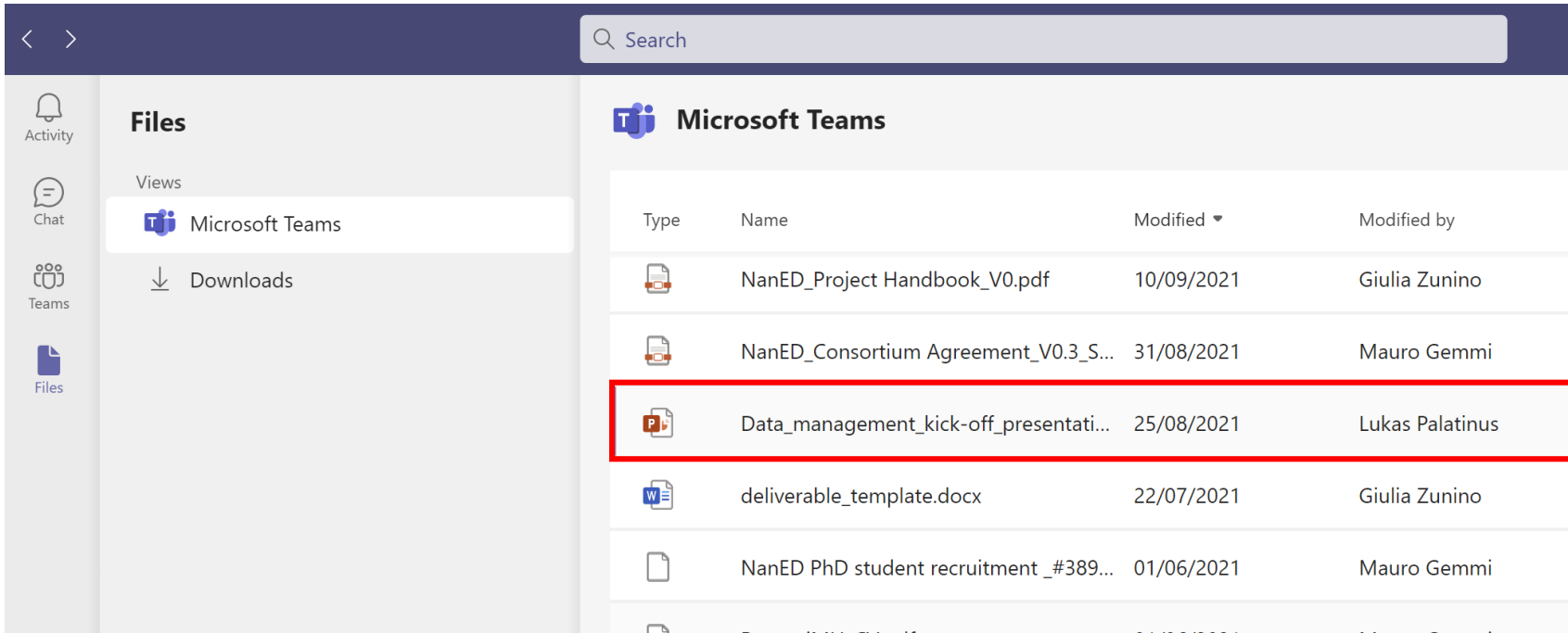
## Conferences specific to your thesis subject:

- Microscopy meetings (**EMC**)
- Material science
- Porous materials, MOF, Catalysis
- Protein conferences
- Pharmaceutical, drug discovery conferences
- Cryo-EM conferences



# Data Repository

## Open data policy by Lukas Palatinus:



The screenshot shows the Microsoft Teams 'Files' tab. On the left, there is a sidebar with navigation icons for Activity, Chat, Teams, and Files. The main area is titled 'Files' and has a search bar at the top. Below the search bar, there are two view options: 'Microsoft Teams' (selected) and 'Downloads'. The main content area displays a table of files. The file 'Data\_management\_kick-off\_presentati...' is highlighted with a red border.

Type	Name	Modified	Modified by
PDF	NanED_Project Handbook_V0.pdf	10/09/2021	Giulia Zunino
PDF	NanED_Consortium Agreement_V0.3_S...	31/08/2021	Mauro Gemmi
PowerPoint	Data_management_kick-off_presentati...	25/08/2021	Lukas Palatinus
Word	deliverable_template.docx	22/07/2021	Giulia Zunino
PDF	NanED PhD student recruitment_#389...	01/06/2021	Mauro Gemmi

- Open science is one of the key concepts propagated by the scientific policy of EU Commission
- Open access – mandatory for all H2020 projects. Green or gold open access
- Open data
  - mandatory for data needed to reproduce and validate the published results
  - optional for all other data



# Workshop at Conferences

## Electron crystallography workshop/school:

- Electron crystallography school at ECM33
  - Organized by Philippe Boullay
- EC School at 26<sup>th</sup> IUCr Congress, Australia
- Erice School of crystallography 2025 (60th Course)
- One special EC school:
  - Organized by ESR
  - ESR as teachers and demonstrators
  - During one **ECM** in collaboration with SIG4 of ECA



ecm33.fr

Versailles, FRANCE

23–27  
AUGUST 2022

33rd European  
Crystallographic Meeting

## Reaching out to other Communities:

An Introductory Course to Three-Dimensional Electron  
Diffraction

12 April 2021 13:00 – 15 April 2021 17:30, United Kingdom 



# Communication Material

## NanED related image and video resources:

- Art galleries (Diffraction patterns, structures, materials, macromolecules)
- Flyers
- Brochures
- **YouTube Videos: Introduction of the projects, lectures, tutorials, results**

## F200

Financement  
100% Région  
**RIN 2019**

**MET-CRISMAT**

*Microscope  
Electronique en  
Transmission pour  
la CRISTallographie  
et la science des  
MATériaux*



### JEOL F200 TEM/STEM CFEG 80-200 kV

Silicon Drift Detector for EDS  
HAADF / ABF detectors  
Tilt range: +/- 30° (**tomo +/- 70°**)  
Digistar + Astar (Nanomegas)



Cryo-Transfer Tomography Holder  
Frost free transfert in TEM at liquid nitrogen temperature

► **hydrated samples, pharma, ...**



+ 1 double-tilt analytical holder + 1 **single-tilt tomography holder**  
+ possibility to use cooling and heating holders already in the lab



4096x4096 fiber-optic coupled CMOS  
max. speed 160 fps (1kx1k); high dynamic range; in-situ mode

► **for image and diffraction**

512x512 Cheetah M3 CMOS hybrid pixel direct electron detector  
max. speed 1750 fps; high dynamic range; no noise

► **for diffraction with high sensitivity in low dose condition**



# Communication Material

## YouTube Videos: Lectures (Examples)

### **cryo-EM**

[https://www.youtube.com/watch?v=gDgFbAqdM\\_c&list=PL8\\_xPU5epJdctoHdQjpfHmd\\_z9WvGxK8-](https://www.youtube.com/watch?v=gDgFbAqdM_c&list=PL8_xPU5epJdctoHdQjpfHmd_z9WvGxK8-)

Credit: Grant Jensen, Caltech

### **Biophysics**

<https://www.youtube.com/user/eriklindahl/videos>

Credit: Erik Lindahl, Stockholm University



# Social Media

**Platform:** Twitter, Facebook, Instagram, YouTube ...

**Purposes:**

- Recruiting
- Training network activities
- Events monitoring
- News/Research news monitoring
- Community building
- Online press relations
- Dissemination

**The dissemination and communication committee will maintain the NanED account**

ESRs are encouraged to run his/her own accounts







# Social Media


## Twitter Example:

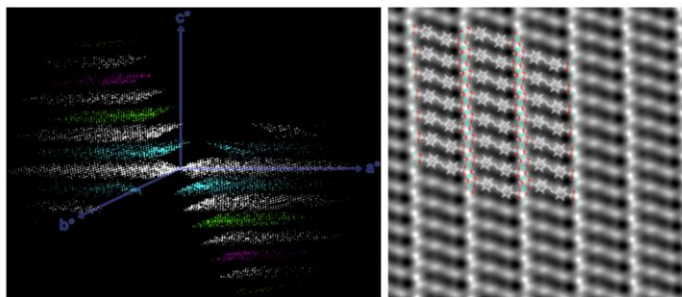
Chirality and accurate structure models by exploiting dynamical effects in continuous-rotation 3D ED data

**Paul Klar** Institute of Physics of the Czech Academy of Sciences; Prague, Czechia,  
**Yasar Krysiak** Institute of Inorganic Chemistry of the Leibniz University Hannover; Hannover, Germany,  
**Hongyi Xu** Department of Materials and Environmental Chemistry, Stockholm University; Stockholm, Sweden  
,  
**Gwladys Steciuk** Institute of Physics of the Czech Academy of Sciences; Prague, Czechia,  
**Jung Cho** Department of Materials and Environmental Chemistry, Stockholm University; Stockholm, Sweden  
,  
**Xiaodong Zou** Department of Materials and Environmental Chemistry, Stockholm University; Stockholm, Sweden,  
**Lukas Palatinus**  Institute of Physics of the Czech Academy of Sciences; Prague, Czechia

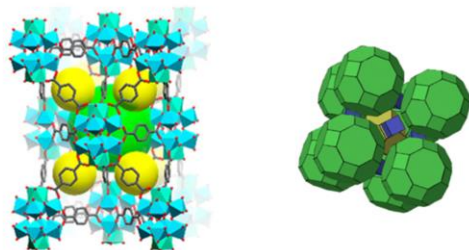
[DOWNLOAD](#) 

**Version History**  
Nov 23, 2021 Version 1

**Metrics**  
 344 Views  
6 136 Content Downloads



Advanced Electron Microscopy



Nanoporous Materials


[Follow @zhehaohuang207](#)

**Tweets by @zhehaohuang207**

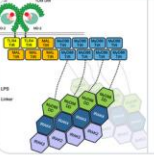
 **IUCr**  
@IUCr  
If you are a young researcher interested in conducting small-molecule single-crystal structure determinations but without access to in-depth training, why not apply to the @IUCr-sponsored Zürich School of Crystallography in June 2022? Deadline 17 Jan 2022 [bit.ly/3c5YZSt](http://bit.ly/3c5YZSt)

**The Zürich School of Crystallography 2022**  
Bring Your Own Crystals  
University of Zürich  
June 19 – 30, 2022  
Organized and directed by  
Anthony Linden and Hans-Benno Bögg

 **Thomas D. Bennett**  
@ThomasDBennett  
Interested in a PhD in Materials Chemistry in Cambridge? Check out the advert below and please get in touch for more details! [findaphd.com/phds/project/s...](http://findaphd.com/phds/project/s...)

 **Max Clabbers**  
@maxclabbers

Our latest manuscript is online, we revealed MyD88 TIR domain higher-order assembly interactions by [#MicroED](#) and [#SFX @XUEY85](#), great collab w/ Bostjan Kobe [@ThomasVe7](#) [@CrollTristan](#) and everyone involved, MicroED highlights summarized below

**nature.com**  
MyD88 TIR domain higher-order assembly interactions reve...  
Nature Communications - MAL and MyD88 are downstream adaptors of Toll-like receptors (TLR) and the MAL TIR doma...

11:49 AM · May 10, 2021 · Twitter Web App

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@maxclabbers

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11:49 AM · May 10, 2021 · Twitter Web App

  
MyD88  
MAL + MyD88  
MAL + MyD88  
MAL + MyD88  
2 µm

  
MyD88 TIR microcrystals, shown here on a vitrified EM grid from 3ul of a 1:60 MAL-MyD88 solution, were typically about 100-200 nm thin, highly suitable for structural characterization by both MicroED and SFX

  
For electron diffraction data collection, we only selected single isolated and still hydrated microcrystals using a 1.8 micron diameter beam (blue) as defined by the selected area aperture on our JEOL 2100 LaB6  
@Stockholm\_Unit  
2 µm



# Newsletter and Blog

## **News Letter (External) – Website**

- 1 news letter per beneficiary – 8 in total
- To be published on the website
- ESRs of the beneficiary will be in charge

## **Blog (Internal) – Microsoft teams, Decide what contents to be included**

- Research highlights
- Research experiences:
  - From the first draft of a manuscript to the published paper
  - How to write scientific paper
  - What to consider when preparing for a presentation
- Personal experiences:
  - Making a breakthrough
  - Attending a conference





# Social Engagement Events

## **Collaborating with the Scientific Culture Units of each host university**

- Science social activities:
  - Science café
  - Science week/nights
  - University open days
  - Science fairs
- Science outreach:
  - Visits to high school / Popular science seminars for school students
  - Host visiting students from schools
  - Popular science article on news papers and magazines
  - Popular science vlog?

## **European Nights of Researchers**

ESRs will participate in the different outreach events organized by each host university



