

# DGK conference 2022



**Monday, 14 March 2022 - Thursday, 17 March 2022**

## Topical tracks

## **Main conference**

### **Covid-19**

#### **Biologic Structure, Function, Reactivity, and Regulation**

macromolecular structures  
methods and facilities  
integrative structural biology  
enzymes  
drug design  
regulation  
complexes  
membrane proteins  
hot structures  
molecular machines  
fold prediction

#### **Structural Chemistry & New crystal structures**

green chemistry  
inorganic crystal structures  
coordination compounds  
small molecules  
organic crystal structures  
supramolecular chemistry  
absolute structure  
polymers  
porous materials (MOFS, Carbons, Zeolites, Polymers.....)  
aperiodic structures  
disorder  
amorphous materials  
nanoparticles

#### **Solid State Physics and Crystal Physics**

magnetism and magnetic structure  
ferroics, multiferroics  
symmetry breaking  
phase transitions  
structure and dynamics  
thermodynamics  
crystal optics

#### **Engineering Materials and Applications**

binders, cement  
battery materials  
in-situ and in-operando studies  
semiconductors  
alloys  
photovoltaics

thermoelectrics  
hydrogen storage  
hydrogen embrittlement  
ionic conductors  
porous materials (MOFs, COFs, Carbons, Zeolites, Polymers.....)  
catalysis  
nanostructuring  
nanoparticles

## **Natural Materials and Environments (Minerals, Biogenic Materials...)**

geomaterials  
biogenic materials  
extreme conditions  
environmental processes  
mineral surface processes  
thermodynamics  
reactivity

## **Structure property relationships**

In-situ and in-operando studies  
extreme conditions  
functional materials  
phase transitions

## **Theory, simulation, modeling, computational crystallography**

group theory  
structural systematics  
electron density  
Hirschfeld atom refinement  
structure prediction  
molecular dynamics  
Monte Carlo  
DFT  
thermodynamics

## **Crystallography in Education, Art, and Society**

science communication  
teaching  
cultural heritage  
science policies  
symmetry and broken symmetry in art

## **Advances in Methods, Instrumentation and Data Analysis**

sources  
beamlines  
optical devices  
sample environments  
data processing  
algorithms and software

artificial intelligence  
electron crystallography  
electron microscopy  
XFEL  
neutrons  
synchrotron  
spectroscopy  
high throughput platforms  
total scattering  
3D delta-pdf

## **Crystallization, Crystal Growth Processes, Synthesis**

environmentally friendly processes  
Crystallography in green chemistry.  
nucleation  
morphology  
microstructure  
defects  
growth mechanisms  
kinetics  
thin films  
surfaces and interfaces

## **Surfaces, Interfaces, Thin Films, Nanoparticles**

surface and interface structure  
reactivity  
catalysis  
nanostructuring

## **Other**

## **Young crystallographers Lightning Talks**