

Inauguration document
Special Interest group of the European Crystallographic Association

Title:

SIG D³ - Dynamics, Disorder, Diffuse scattering

Promoters:

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Proponents:

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Founding members:

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Scope and Objectives:

SIG D³ brings together scientists working on dynamical properties, disorder and diffuse scattering. The main objectives are to enhance the exchange of information regarding recent progress in experiment and theory, to provide a platform for discussions, to promote use of diffraction and crystallographic tools in studying the physics and chemistry of materials which display some kind of disorder.

SIG D³ aims at achieving a coherent understanding of the various contributions to Bragg and diffuse scattering related to disorder phenomena. The disorder is taken here in a broad sense and includes structural imperfections present at different time and length scales, varying from domain walls to compositional fluctuations and fundamental excitations in non-ideal crystals. We note that this field has experienced a significant revival thanks to the advent of bright synchrotron and neutron sources, the development of new detectors, and the availability of powerful computing tools. SIG D³ also focuses on experimental techniques to probe disorder and dynamical response, and on the processing and presentation of big data sets associated with the study of diffuse scattering. SIG D³ also aims at generating a pool of software and experimental facilities best suited for studies of dynamics and disorder phenomena.

At present, the following topics play an important role in the field:

- Diffuse scattering associated with fundamental excitations
- Atomic displacement parameters and lattice dynamics
- Ab-initio calculations of lattice dynamics and thermal diffuse scattering

- Occupational, displacive, and orientational disorder in crystals
- Correlation analysis of diffuse scattering
- Extracting 3D pair distribution functions from diffuse scattering
- Direct space modeling of disordered systems with Monte Carlo and other techniques
- Disorder in photonic crystals
- Magnetic diffuse scattering
- Dynamics and disorder at extreme conditions
- Excited state crystallography
- Inelastic X-ray and neutron scattering
- Diffuse scattering in powder diffraction
- Macromolecular diffuse scattering and dynamics of proteins

Membership:

All European scientists interested in dynamics, disorder and diffuse scattering are welcome to join SIG D³. Participation requires ECA membership.

Organisation:

The activities of SIG D³ will be organized by its Steering Committee, consisting of maximal eight members (including Chairperson, Vice-Chairperson, Secretary). The steering committee will be elected/confirmed during the ECM's.

(Preliminary) rules of the SIG:

After approval of the SIG, the membership of the SIG is open to all European crystallographers active in the field of crystallography of disorder, diffuse scattering and dynamic phenomena. It is intention of the promoters to have a meeting of the Founding members and other interested crystallographers at 31st European Crystallographic Meeting, ECM31, in Oviedo, Spain, 2018. In this meeting more formal rules should be established and officers of the SIG (chairman, vice-chairman, secretary) should be formally elected. Till that time, the promoters shall act as contact persons with ECA (Björn Wehinger, Dmitry Chernyshov, Anders Østergaard Madsen).

Activities

- Organisation of Micro symposia and plenary talks during ECA meetings
- Independent workshop and satellite meetings of ECMs
- Schools for young scientists
- Website with links to specialized literature, data analysis programs, databases and announcements of activities and open positions within SIG-D³.