

## 18. Gervais Chapuis

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*Incommensurate crystals / Diffraction studies /  
Molecular dynamical modelling /  
Crystallographic teaching*

### 1. What is crystallography?

Crystallography is essentially the study of the structure of matter on the atomic scale and its relation to macroscopic properties. In this definition, we strictly avoid the use of crystal in order to reflect the ever increasing role of other forms of condensed matter. The relation to macroscopic properties reflects the role that crystallography can play in basic sciences and in the development of new technologies.

### 2. Is there a better name that could replace the historical term “crystallography”?

Without doubt, the field of crystallography has greatly evolved in the past decades and is still continuing to do so. Unfortunately, this evolution has not been reflected in the perception from the community external to the field. Even among crystallographers, not to mention other specialists, the confusion between “diffraction” and “crystallography” is a true indication of the misunderstanding of its nature. It is probably difficult to change the name which is well established. However the crystallographer’s community should better promote the image of their rapidly evolving speciality. Perhaps the most important is the need to clearly differentiate between crystallography as a basic science and its commercially successful aspects which are inevitably better known.

### 3. What are the most important unsolved problems in crystallography?

In the past, crystallographers have dedicated their efforts mainly to the structural characteristics of matter. In the future, their research should be oriented towards a better understanding of the relationship between structures and macroscopic properties such as physical, chemical and biological. Understanding the relationship between structures and functions or the structure of transient or excited states are examples of future challenges for crystallographers.

### 4. What is the future of crystallography?

The rapid development of new sources of radiation and detectors is a unique opportunity for crystallographers to regain the spirit of pioneering research which they enjoyed in the first half of the past century. The ability to record, in ever shorter period of time, the complete spectrum of a diffracting object and exploit it, is a challenging opportunity to give a new momentum in crystallographic research. The combined study of diffracting systems under dynamical conditions will without doubt influence the research in the years to come.

Crystallographers will have to take into account simultaneously both aspects of real structures, *i.e.* the periodicity of structures and all types of deviations from this order. It is only through these combined consideration that crystallographers will be able to contribute to the challenges of unsolved problems. Not only the phenomenon of diffraction should be considered for investigation but also various aspects of scattering and absorption processes should be accounted for in order to get better insight into the properties of condensed matter.

Ultimately, crystallography will reach the limit in space (single molecule study) as well as the limit in time (time resolved study).

### 5. Should we still teach crystallography?

The teaching of crystallography should reflect the vision and the evolution of the field. The topics which have been taught in the past are much too narrow and often failed to attract curious students. The topics should definitely be enlarged and include neutron, electron diffraction and other relevant scattering processes. Efforts should be made to develop pedagogically oriented websites not only to attract students but also to compensate for the curricula where less and less time is dedicated to the field of crystallography.

### 6. Personal recommendation to a student who wants to enter into crystallographic research

Crystallography is a modern science with a notorious interdisciplinary character with applications in basic and applied sciences. The development of new powerful instrumentation of the latest generation requires new theoretical and experimental approaches. For the students, this opens a large spectrum of future research possibilities ranging from theoretical physics to applied natural sciences. Crystallography plays a key-role in many industries and therefore, the education of crystallographers is crucial.

### 7. What is the impact of crystallographic research?

There is a clear trend in science and engineering to evolve from a purely descriptive approach towards the understanding of macroscopical phenomena and of the microscopic behaviour of materials. Crystallography is the key

discipline for elucidating microscopic structure. The engineering of new materials with specific properties is based on the knowledge of microscopic structure. Crystallography is the fundamental discipline, which provides us with this knowledge.