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Exploring structural biology on the web: to biologists and beyond

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Teaching macromolecular structure is often complicated by the need to have specialist tools to view structures and related information. At the PDBe we have integrated a number of different components that allow easy visualisation of structural data in different ways within the web browser.

These components include lightning-fast molecular visualisation with LiteMol and a sequence component to link this visualisation to the primary structure, via secondary structure topology diagrams. These interactive components enable students to explore sequence information and its relationship to 3D structure. The components integrate extra annotations including domains and validation data. Visualisation of electron density maps within LiteMol makes it an excellent tool for introducing students to the importance of validation in structural biology.

All of these components operate within a browser window, including on mobile devices, meaning that they are available to anyone, anywhere. This has enabled us to effectively teach macromolecular structure to students at all levels and even to introduce structural biology to artists and the wider general public. We hope this will help to bring structure to biology and beyond.

References:

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Keywords: Visualisation, Sequence to structure, validation

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A model description of crystalline state under external influences

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A method is proposed for describing the change in the ground state of a phase of a crystalline substance under external influences. This manner of expression takes into account the multifactorial nature of governing factors which determine phase transitions and influence the functional characteristics of the materials being created from the substances. The phase space for crystals is constructed vector interactions) using three basic and enough independent factors and then associated with the composition of substance. They describe, first, the change in the level of available potential or the incoming energy to the substance; second, the time characteristics, included for describing emerging and existing phases; third, the spatial localization of the phase, respectively.

For a more detailed description of the processes of phase state change under external influences these factors consistently combine into the factors of the second level, which create subsystems to describe the origin of space-time patterns, the evolution of the state of the phase, and third, to describe the phase transitions in substances. Then a subsequent combination of all three specialized second-level factors in the third-level factors makes it possible to describe the relationship of changes in composition and structure with functional characteristics that reflect the generalized information nature of these characteristics; this can be used to describe more complex behavior, for example, temporal oscillations of all structural parameters in certain inorganic, usually multi-component substances.

The use of the model in educational practice has shown that the proposed method of description of a crystal phase state is useful for a more accessible and comprehensive, and also for a wider explanation of the multifactor nature of characteristics of condensed substances in the crystalline state. The model also ensures a better transfer of the accumulated knowledge about the specific features of the crystalline state into the processes of creating and developing new types of crystals and the technologies for the production and processing of materials, necessary for use in various spheres of life and industry.

The connection of this model with fundamental physico-chemical concepts can be useful for students as a new tool for deeper and successful mastering of crystallography. We noticed [1-3] that students whose crystallographic interests are related to the functional information properties of substances based on the key factors of the crystalline state, faster socialize in the modern information society and more confidently and reliably solve specific problems in the field of materials science.

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The crystallization competition in the school: an innovative teaching/outreach tool for secondary schools

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The 'Crystallization Competition in the School' is a teaching/outreach activity aimed at students aged 12-17, whose main goals are to disseminate the importance of crystallography and crystallization and inspire scientific vocations. Since it was first organised in 2009/2010 (Andalucía/Puerto Rico), the popularity of the Competition has quickly spread across Spain. In this school year (2017/2018), eight editions have been organised in different regions of Spain, counting with the direct participation of 282 schools, 495 teachers and 7,768 pupils.

The format of the Competition is intended to provide school students the experience of being a 'real' scientist: from designing a scientific project, through working in practical crystallization experiments and keeping a laboratory notebook, putting into practise their presentation skills and sharing outcomes with scientists and fellows from other schools. This innovative approach is implemented in three successive stages that place teachers at its heart in order to engage with the entire educational community. At the first stage, teachers are trained in fundamental crystallography and crystallization concepts through the organisation of a practical workshop that provides them with teaching tools and resources that can be turned into enjoyable activities for the classroom. In the second stage, students develop a laboratory project under the supervision of their teachers making use of a motivating crystallization kit of ammonium dihydrogen phosphate (ADP) that enables them to stir their scientific imagination and bring out their scientific spirit. Students can also develop other types of projects such as crystallization of salts by cooling, formation of geodes and crystallization in gels. The final phase of the Competition is organised similarly to a scientific conference, where students make the presentation of a poster, their grown crystals and a lab notebook that is evaluated by a panel of scientists. By the end of the Competition, students will have learnt to behave as 'scientists' and developed work-related scientific values such as observation, systematic study, rational thinking, teamwork and communication skills.