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The Crystallogame

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X-ray crystallography has been developed as the main experimental technique to investigate the 3D structure of proteins, giving knowledge at atomic resolution of the molecular details of macromolecules. Nevertheless, still many people even among the scientific community ignore the basic principles of X-ray crystallography that allow to use a diffraction pattern to build the electron density map used to derive a 3D model of a molecule. Here we present The CrystalloGame, a prototype of puzzle-game based on the phenomenon of X-ray diffraction which proposes the main aspect of crystallography in a playful way.
This videogame is structured as a sequence of levels of increasing difficulty, each consisting of a puzzle to be solved. Actually, the videogame is equipped with an interface that allows the player to modify the 3D configuration of a crescent number of atoms in search of the correct spatial disposition that produces a given diffraction pattern. For this purpose, we developed an algorithm able to reproduce the interference pattern generated by a configuration of the atoms, simulating the real phenomenon with a certain approximation. The simulation is operated by a GPU software in order to guarantee the computational efficiency necessary for the execution in real time during the game. Many important aspects that characterize a real diffraction experiment are introduced in the videogame in form of power-ups available at different levels, for instance the possibility to modulate the X-ray wavelength, the ability to rotate a fixed atomic configuration and the introduction of atomic repetitions simulating a crystalline structure.
The aim of this videogame is to guarantee a gradual understanding of the aspects underlying X-ray diffraction experiments and to stimulate the player to verify through direct experience how a diffraction experiment works.
Hopefully, The CrystalloGame will contribute to the dissemination and popularization of crystallographic sciences by fascinating a new generation of desirable future crystallographers.
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