(COKAT) Development of a crystallographic interface for Blender

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Masterproef bij:

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Doelstelling:

Science not only depends on top level research but critically hinges on concise communication of results. One of the most potent means to share scientific insight are high quality graphics. This is especially true in the field of crystallography, where a single image can convey a message which would otherwise require pages of convoluted text.
Many programs exist which can display crystal structures in 3D. However, none of these has the full range of 3D virtual reality options current graphics software and game engines provide. One program being extremely flexible and powerful in terms of graphical design is Blender (www.blender.org). Most importantly, Blender is an open source project, licensed under the GNU GPL. All code is written in C, C++ and Python. It is well documented, offering a comprehensive application programming interface (https://docs.blender.org/api/blender_python_api_2_77_0/info_overview.html), and content can easily be executed in Blender either as script or as interactive addon.
The task for the here proposed project is the creation of an interface, which allows the direct import of crystallographic content into Blender.

Beschrijving:

Proposal

After a first exploration of Blender, its structure and functionality, the student will be introduced to the way how crystallographic content is stored in a crystallographic information file (cif). Special attention will be given on how a transformation of crystallographic coordinates can be transformed to the Cartesian system. The first milestone of the thesis will be the generation of one crystallographic unit cell, containing all provided atoms, in Blender. Asides subroutines for coordinate transformation this also involves concise design of classes allowing sufficient flexibility for further functionality. This first milestone will provide the direct option to display crystal structures and at the same time will train the student in the data structure of Blender vs. crystallography. During this stage of development the student will be guided in correct analysis of geometric relation between real space and crystal space.
The second milestone then will involve the introduction of the crystal symmetry, i.e. the generation of symmetry equivalent atom sites related by symmetry operations, like mirror operations or rotations. Libraries which contain the necessary routines to generate full structures from spacegroup information are available and need to be linked to the developed code (https://cci.lbl.gov/cctbx_docs/cctbx/cctbx.html).
The third milestone will be the introduction of editing tools of the structure imported into Blender. This includes the option to display specific regions defined either by specification of a box in crystallographic units or a sphere around a special atom or coordinate. Also tools involving the option to select atoms, either by name, type or by cursor need to be devised. Furthermore, tools to create and edit bonds and polyhedra based on user provided specifications (e.b.: bond distances) should be developed. For the latter, preliminary routines already exist.

This masterproject occurs in collaboration between the Centre for Surfacechemistry and catalysis and Electrical Engineering (ESAT) TC.
The project will focus on program development in Python and C++. A basic knowledge in physics and crystallography on bachelor level is useful, but not necessary as all required knowledge will be provided.
Close tutoring is foreseen personally and also via Skype to allow fast progress.

Remarks / Opmerkingen

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Assistants