Infinity and beyond – using virtual reality to teach space group symmetry and periodicity

N. Graw, M. Mücke, A. Krawczuk

Georg-August-Universität, 37077 Göttingen, Germany
ngraw@chemie.uni-goettingen.de

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Unarguably, space groups are among the more complicated symmetry considerations students must tackle during their studies of natural sciences. Yet they are of utmost importance to understand structure property relations and to design new materials with tailored properties. Since space groups are three-dimensional arrangements of symmetry elements, it requires spatial imagination to understand them. Two-dimensional notations, such as those used in the International Tables of Crystallography, Section A[1] are a great tool for trained crystallographers but require a high degree of visuospatial thinking from beginners. To help students develop a better understanding of space groups we designed physical three-dimensional models of whole unit cells, which explicitly depict symmetry elements and allow to comprehend how symmetry determines the arrangement of e.g. molecules inside the cell.[2,3]

However, such physical models have two major drawbacks. First of all, they are usually only available during lectures or seminars. Hence, they are of no use during self-study or for exam preparation. Secondly, for practical reasons physical models are often restricted to one unit cell or only a very limited number of them. This circumstance prevents such models to adequately address periodicity albeit being a core feature of solid-state structures.

To remedy this situation, we prepared digital three-dimensional models of unit cells which can be viewed in virtual reality (VR), while the interactability of a classical physical model is retained. The VR models of singular unit cells are 360° accessible and help to grasp the three dimensionality of solid-state structures. Visualisation can be changed between unit cell contents and symmetry elements (or both) depending on what is more appropriate for the topic to be discussed (see Fig. 1). Furthermore, this approach allows a model of a single unit cell to be extended to a virtually infinite lattice and generates an immersive teaching experience for students as these can observe the crystal structure from within.

Figure 1. Different visualisations of a unit cell showing only the symmetry elements (left), symmetry elements and molecular content (middle) or only molecular content (right).


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