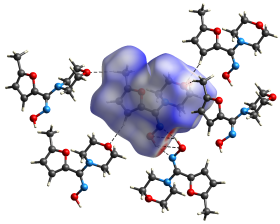

Figure 1. The Hirshfeld surface mapped with d_{norm}

Keywords: Single crystal X-ray diffraction, Density Functional Theory, Hirshfeld Surfaces, Spectroscopic Methods

MS47 Teaching & Education

Chairs: Helen Stoeckli-Evans, Howard Flack

MS47-P1 Modern web technologies as tools in teaching crystallographic group theory

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The concept of symmetry is central to crystallography. Although symmetry is ubiquitous around us, it takes some conceptual effort to leverage this everyday knowledge in understanding why the molecules pack the way they pack in crystals. Group theory on the other hand is a mathematical formalism describing symmetry. In the crystallographic context it comes in the form of point, plane and space groups. As with any abstract concept to be learned, it is easier to understand by visualization.

Today there are plenty of excellent libraries for visualization of data in 2D (like for example d3.js[1]). Even the HTML standard has evolved in the way that it now natively supports drawing on its canvas. Combined with some great capabilities of the general purpose library for crystallographic computations such as cctbx[2] it can be used to bring the visualization of space group patterns to a very broad audience, practically everyone and everywhere. This undertaking was conceived originally as a help in teaching the course "Group theory in crystallography" to graduate students of chemistry.

1. https://d3js.org/

2. R. W. Grosse-Kunstleve, N. K. Sauter, N. W. Moriarty and P. D. Adams, *J. Appl. Cryst.* **35** (2002) 126-136.

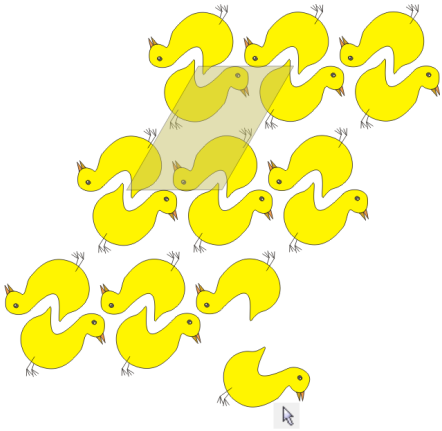

Figure 1. Trying to arrange objects interactively in „crystal“ packing can be more instructive than learning group theory formalism just through theorems and formulas.

Keywords: teaching group theory, web visualization,

MS47-P2 Crystallography through children's literature: The Curious Monster book series.

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The Curious Space is an Early Childhood Science Program developed at the University of Oviedo [1]. The main objective of this project is to engage children on science discovery and to help to foster science vocations.

From a very early age, children have the basic abilities for science learning and performing. Indeed, from birth children have the propensity to observe, explore and discover the world around them. These abilities should be supported and encouraged by exploratory play and other forms of active engagement [2]. Picture books are really effective for engaging readers of all ages and building scientific inquiry [3]. In *The Curious Space* children learn science concepts by reading picture books, doing a number of experiments and interacting with scientists.

Regarding crystallography, we have published the children book's series called **"The Curious Monster"**. This is a set of three picture books that **bring crystallography closer to the youngest readers**. Each book of the series addresses different aspects and concepts of crystallography and scientific communication and pretends to give an in-depth coverage of them. In *The Curious Monster and the Carbon Stars*, concepts such as particles, crystal, polymorph and structure are introduced. In the second book of the series, *The Curious Monster and the Ring of Light*, synchrotron radiation and its applications on crystallography are introduced. The last volume of the series, *The Curious Monster and the Mysterious Stone*, is an introduction to science communication and conferences. It also introduces and reinforces valuable crystallography concepts such as rock, mineral and crystal.

The Curious Space activities about crystallography are designed for working with children ages 4-9. The workshops start by reading aloud one of the Curious Monster book. This stimulate children on both the emotional and intellectual levels. Children easily connect with the personality and adventures of the characters, and feel fascinated by the science that supports the stories. The reading experience is paired with a practical experience, in which the students actually touch and make science.

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References: [1] http://elmonstruocurioso.org [2] National Science Teachers Association (2014). *NSTA Position Statement: Early Childhood Science Education.* [3] *Acta Cryst* (2015). A71, s527-s528.

Keywords: Teaching crystallography, science vocations, children's literature