

## Microsymposium

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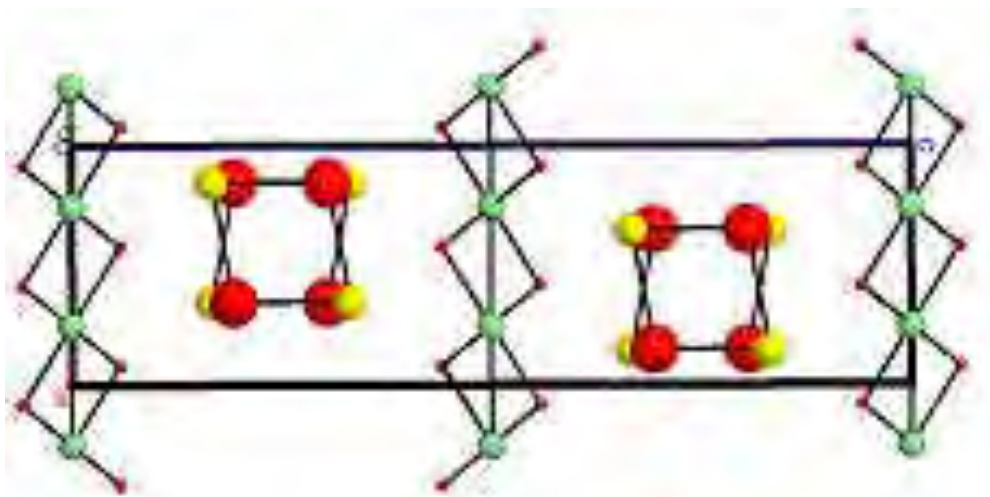
### *New Methods for the Visualization of Incommensurately Modulated Structures*

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While the theory of incommensurate structure and composite crystallography is well established, methods for the visualization of modulated and composite crystal structures are few.[1] At the same time, databases featuring such structures have arisen [2], and there is a growing need for web-based tools that allow users to interactively explore such structures. This presentation is by the principal developer of Jmol, an international open-source collaborative molecular visualization project. It will focus on recent developments that have been made in this area. Jmol provides a flexible and crystallographically rich suite of functionality, including depiction of specific symmetry operations and selective sets of unit cells, selection of specific modes of modulation, use of color to show long-range low-frequency modulation components, and the depiction of relative modulation phasing through animation. From an archival perspective, Jmol development has been an opportunity to test the basic ontology of the IUCr msCIF standard [3], and a number of issues relating to this standard will be discussed, particularly in relation to multidimensional modulation. From an general educational perspective, Jmol for the first time allows easy access to a wide variety of examples of incommensurately and commensurately modulated structures and composite structures. Being accessible on virtually all platforms and within all major browsers, Jmol offers a novel mechanism for the wide-spread dissemination of understanding of this important class of crystal structure.

[1] [a] Jana2006, Petricek, V., Dusek, M. & Palatinus L. (2006) [<http://jana.fzu.cz/>], [b] Jmol, Hanson, R., et al. [<http://jmol.sourceforge.net/>], [2] [a] B-IncStrDB - The Bilbao Incommensurate Structure Database [<http://b-incstrdb.ehu.es/incstrdb>] [b] Powder Diffraction File, International Centre for Diffraction Data [<http://www.icdd.com>], [3] International Tables for Crystallography, Volume G: Definition and exchange of crystallographic data, Edited by S. R. Hall and B. McMahon



**Keywords:** visualization, incommensurate, modulated