KN14 **Charge Densities and Crystal Engineering**

Mark A. Spackman, *School of Chemistry & Biochemistry, University of Western Australia, Australia*
E-mail: mark.spackman@uwa.edu.au

The development of molecular crystalline materials with desired chemical or physical properties underpins many technological advances. Successful design of these materials demands knowledge and understanding at three different levels:

- the structure and properties of the constituent molecules;
- how these properties lead to observed crystal structures; and
- the relationship between molecular properties and those of the bulk material.

Many different aspects can be identified with each of these levels of understanding. For example, computational chemistry and experimental charge density analysis can provide information on molecular properties. Crystal structure prediction typically uses theoretical models for molecular charge distributions (in the form of atomic charges and multipoles, or as a discrete pixellated breakdown of the electron distribution) to evaluate the electrostatic components of interaction enrgies.

Our research in recent years has touched on aspects of all three of these levels, especially the relationship between molecular properties, crystal structure and bulk properties. The common thread in all of our studies has been a detailed appreciation of the nature of the molecular electron distribution. We are particularly interested in how and where it differs from that due to a simple sum of spherical atoms (the promolecule), and devising ways in which the two can be used together to facilitate understanding of *how* molecules pack in crystals, *why* it makes sense that a particular crystal packing occurs, and *what* can be learned about the bulk in this manner.

This presentation will provide an overview of our latest research involving Hirshfeld surface analysis,[1] electrostatic complementarity [2] and the mapping of void space in molecular crystals.[3]

[1] Spackman, M. A. & Jayatilaka, D. (2009). *CrystEngComm* 11, 19-32.
[2] Spackman, M. A., McKinnon, J. J. & Jayatilaka, D. (2008). *CrystEngComm* 10, 377-388.
[3] Turner, M. J., McKinnon, J. J., Jayatilaka, D. & Spackman, M. A. (2011). *CrystEngComm* 13, 1804-1813.

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