

Rings and Chains in Solid-State Chemistry. The Electron Count Matters

Jean-François Halet

Institut des Sciences Chimiques de Rennes, UMR 6226 CNRS-Université de Rennes 1, F-35042 Rennes, France. E-mail: halet@univ-rennes1.fr

There is value in considering a solid as a molecule, a big one, but just a molecule [1]. Both molecules and solids deal with the same fundamental questions: Where are the electrons, where are the bonds? A few examples of solid-state compounds will be discussed, borrowed from the metal boron or metal boron carbon chemistries [2]. They will serve to illustrate similarities (and differences) between the bonding in molecules and solids. Parameters such as the symmetry, the electron count and the nature of the chemical elements will be analyzed with the aid of molecular and periodic density-functional theory tools to address the issues of structural arrangement and physical properties of examples containing non-metal rings and chains [3]. A comparison with molecular chemistry will be made.

[1] T. P. Fehlner, J.-F. Halet, J.-Y. Saillard, *Molecular Clusters. A Bridge to Solid State Chemistry*, Cambridge University Press, Cambridge, UK, 2007.

[2] a) J. Bauer, J.-F. Halet, J.-Y. Saillard, *Coord. Chem. Rev.* **1998**, 178-179, 723-753. b) M. Ben Yahia, J. Roger, X. Rocquefelte, R. Gautier, J. Bauer, R. Guérin, J.-Y. Saillard, J.-F. Halet, *J. Solid State Chem.* 179 (2006) 2779-2786. c) T. Mori, in: K. A. Gschneidner Jr., J.-C. Bunzli and V. Pecharsky (eds) *Handbook on the Physics and Chemistry of Rare Earths, Higher borides*, North-Holland, Amsterdam, 2008, p. 105-173.

[3] a) X. Rocquefelte, S.-E. Boulfelfel, M. Ben Yahia, J. Bauer, J.-Y. Saillard, J.-F. Halet, *Angew. Chem., Int. Ed.* **2005**, 44, 7542-7545. b) J. Cuny, S. Messaoudi, V. Alonzo, E. Furet, J.-F. Halet, E. Le Fur, S. E. Ashbrook, C. J. Pickard, R. Gautier, L. Le Polles, *J. Comput. Chem.* **2008**, 29, 2279-2287. c) S. Lassoued, R. Gautier, A. Boutarfaia, J.-F. Halet, *J. Organomet. Chem.* **2010**, 695, 983-997. d) S. Lassoued, R. Gautier, J.-F. Halet, in *Boron Rich Solids: Sensors, Ultra High Temperature Ceramics, Thermoelectrics, Armor*, Eds. N. Orlovskaya, M. Lugovy, Springer Science and Business Media V. B., 2011, pp. 95-114.