

Electron density in molecules under high pressure

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The research on molecular crystals under high pressure is growing at an exceptional rate given that this field was largely unexplored. Molecular solids under pressure offer a glimpse of the effects of raising the internal energy of a system. Noteworthy, the energies of the electronic ground state and of the excited states do not change homogeneously while the lattice shrinks. Therefore, the degree of contamination of higher energy electronic states may increase upon compression.

This could lead to unusual electronic configurations, switch between specific electronic states (especially in metal complexes), activated molecules and, in the most intriguing case, products of a chemical reaction. Each of these transformations is characterized by specific changes of the distribution of electronic charge in the molecule and sometime also a different spin density distribution.

In this talk, some examples¹ will be illustrated of the enormous information provided by electron density analysis in solids under high pressure. The methods to determine experimentally the electron density at these extreme conditions will be also discussed.

¹ a) Macchi, P.; Casati, N.; Evans, S. R.; Gozzo, F.; Simoncic, P.; Tiana, D. *Chem. Comm.* **2014**, 50, 12824 – 12827; b) Lanza, A.; Fiolka, C.; Fisch, M.; Casati, N.; Skoulatos, M.; Rüegg, C.; Krämer, K. Macchi, P.; *Chem. Comm.* **2014**, 50, 14504-14507; c) Scherer, W.; Dunbar, A. C.; Barquera-Lozada, J. E.; Schmitz, D.; Eickerling, G.; Kratzert, D.; Stalke, D.; Lanza, A.; Macchi, P.; Casati, N.; Ebad-Allah, J.; Kuntscher, C. *Angew. Chem.* **2015**, 54, 2505 –2509