

Topological partition of the elastic constants of crystals

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In a previous work, we have shown [1] the QTAIM (Bader) partition of the elastic constants into atomic components, based on the volume partition of the basins. We have also discussed how this volume partition is complementary but different to the energy partition of the same elastic constants. Tsirelson et al. [2] have explored different electron-density -based energy functionals of the energy and in this communication we will try to apply their experience to advance in our subject. Furthermore, Yu and Trinkle [3] have shown that solving the difficult problem of determining the basin surface is not required to integrate the electron density within the QTAIM basins if the density is represented on a uniform grid.

References:

- [1] A. Otero-de-la-Roza and Víctor Luaña, *J Phys Chem A* **115** (2011) 12953.
- [2] V.G. Tsirelson and R.P. Ozerov, *Electron density and bonding in crystals* (IOP, 1996).
- [3] Min Yu and Dallas R. Trinkle, *J. Chem Phys* **134** (2011) 064111