Crystals Compressibility and Quantum Electronic Pressure

Yury Matveychuk[1], Sergey Sobalev[1], Ekaterina Bartashevich[1]

[1]) South Ural State University, Chelyabinsk, Russia
matveichukyv@susu.ru

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We performed the relationships between quantum electronic pressure[1] (QEP) and spatial dependences of crystal compressibility on the examples of MgB_2 and C_6Hal_6. Crystal's compressibility of two types was considered: under uniaxial stress (Young's modulus) and hydrostatic stress (linear compressibility). The crystal stiffness tensors for calculation of elastic moduli were obtained by DFT calculations with periodic boundary conditions using CRYSTAL17 software. Calculations of QEP were performed using WinXPRO 3.4.29 and 3DPlot programs[2]. Anisotropy of compressibility decreasing under external pressure is correctly matched with the QEP changes along bond paths and in other regions of crystal structures.

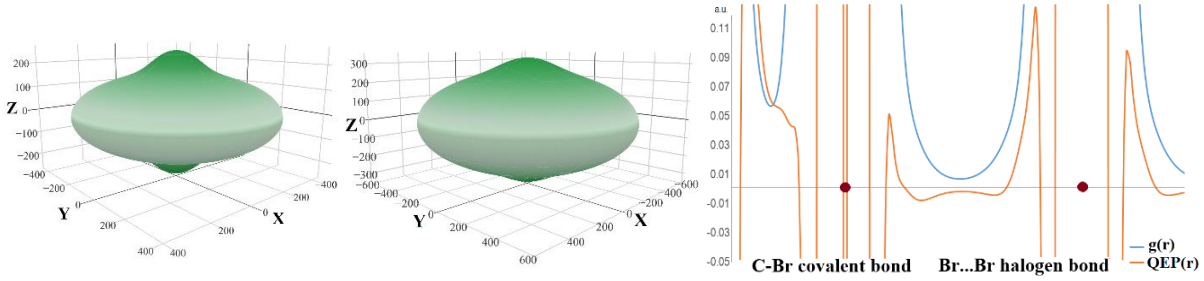

Figure 1 a) Young's modulus of MgB2 under 0 and 20 GPa of external pressure; b) QEP and the density of kinetic electron energy g(r) for Br…Br halogen bond in C_6Br_6 crystal

In a crystal, the regions of negative QEP indicate that the quantum contribution to the local internal energy of electrons is ready to compensate the stress growing under external pressure. Along these regions arrangement, the maximal crystal compressibility is observed, namely along the stacks in C_6Hal_6 crystals and orthogonally to the B atom and Mg atom layers in MgB_2 crystals. The regions of positive QEP show the largest resistance to external stresses and exhibit the least geometric changes under external pressure, like B–B bonds in MgB_2. The halogen bonds forming Hal_3-synthons in C_6Hal_6 determine the decreasing crystal compressibility in the directions parallel to these bonds in the series Cl > Br > I, which is clearly related with the negative QEP decreasing in the regions of halogen bonds.

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