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Negative compressibility: mechanism in Platinum Sulfide

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Abstract – New quantum mechanical calculations on the material PtS not only identify alternative structures but show that this material could be one of the very few to expand in one direction when submitted to isotropic pressure, with possible applications in high pressure environments, sensors or filters.

Materials with unusual elastic properties have been known for a long time —in 1957, J.F. Nye [1] mentions that Tellurium exhibits negative linear compressibility (NLC)—, but have only received extensive interest following works on auxetic properties (negative Poisson's ratio). While auxetic materials are relatively common [2], only fourteen examples of materials with NLC have been found [3]. Possible applications include filtration, sensors and incompressible structures. I have studied the structural, elastic and dynamic properties of the mineral cooperite, PtS (tetragonal, space group P42/mmc [4, 5]) under pressure using Density Functional Theory with different combinations of pseudopotentials and functionals. The results show: a competition with the less symmetric but more compact PdS structure, an associated anomalous elastic behavior where PtS expands along its long axis under hydrostatic pressure —exhibiting NLC—, and a soft mode at (.5,.5,0), corresponding to a doubled, slightly more stable structure —still exhibiting NLC—.

While LDA calculated lattice parameters agree more with experimental results, with this functional the material crystallizes in the related but denser PdS structure (Fig. 1). On the other hand, the GGA functional stabilizes the original PtS structure, and estimate the pressure at which the PtS/PdS transition occurs at 4GPa, to 1GPa of its experimental value [6].

Below the phase transition pressure, all combinations show that PtS displays anomalous elastic behavior by expanding along its long axis under hydrostatic pressure (Fig. 2). This phenomenon does occur for all functionals, and can be linked with a phenomenological interpretation of the phase transition and interpretation of the experimental lattice parameters,

I will also present the ElAM computer code (Elastic Anisotropy Measures), which can represent a variety of elastic properties in any direction (Fig.3), and is a powerful tool to identify abnormal behavior.

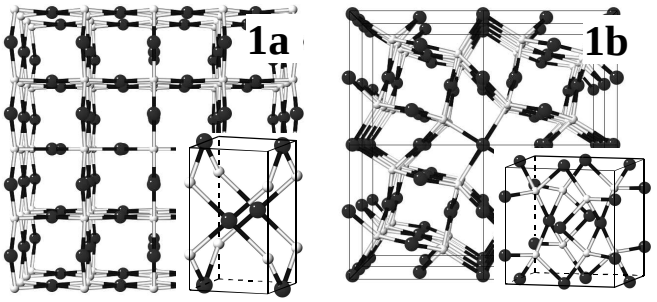

Figure 1: (a) Structure of PtS, (b) Structure of PdS. Small white sphere: sulfur atom, large black, platinum. The main figure shows a projection on the [001] plane, the insert represents the primitive cell.

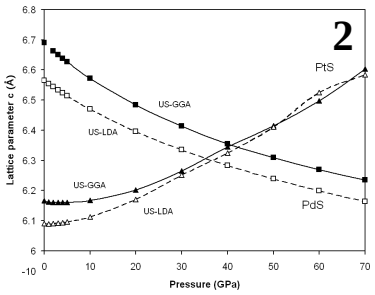

Figure 2: Lattice parameters c of the PtS (triangle) and the PdS (square) structures as a function of pressure for US-LDA (broken line, empty symbols) and US-GGA (full line and symbols) calculation.

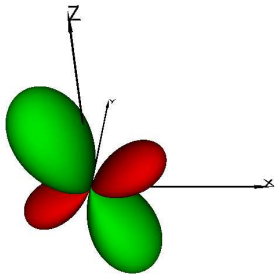

Figure 3: 3D representation of the linear compressibility of monoclinic LaNbO4. The surface represents the amplitude of LC for each direction; positive (green/clear) and negative (red/dark).

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