Can standard DFT calculations correctly describe the physical properties of AlOOH under pressure?

Cortona P
University of Paris-Saclay, France

The behaviour of AlOOH under pressure has been the object of many experimental studies. Under ambient conditions, AlOOH is stable in the α phase (also called diaspore). The δ phase becomes the stable phase at about 17 GPa, while a third phase (called γ phase or boehmite) is metastable. These three phases differ for the arrangement of the oxygen octahedra surrounding the Al atoms and for the kind of hydrogen bond connecting the octahedra.

AlOOH equations of state have been reported in various papers, but, even when the p-V data collected by different researchers agree quite well, the bulk moduli obtained by fitting the data with Birch-Murnaghan or other analytical equations of state are very different. Quite strangely, large discrepancies are also found among the theoretical results, even if the calculations have been done using the same approximations.

I will discuss the origin of these uncertainties by mean of DFT calculations. Furthermore, I will show that the use of GGA for solids (like PBEsol or TCAsol) is mandatory to obtain a satisfactory and quite accurate description of this system. I also discuss the symmetrisation of the hydrogen bond in the δ phase. There is a long-standing debate about the pressure at which the symmetrisation of the hydrogen bond takes place. I will show that PBEsol and TCAsol allow one to come to a quite convincing and well-defined conclusion.

Speaker Biography

Cortona P is professor of physics at University of Paris-Saclay, France. His research domain is mainly the density functional theory and its applications to solid-state and surface physics. Among his more recent achievements it can be mentioned the PBE0-1/3 hybrid and the TCA and SG4 GGA functionals. He was the author of the so-called density-functional theory for subsystems.

e: pietro.cortona@centralesupelec.fr

Notes: