First-principles calculations of the electronic structure, optical and mechanical properties of 21 chalcogenide crystals: Ag2S, Ag2Se, Ag2Te, As2S3, As2Se3, As2Te3, As4Se4, Cu2S, Cu2Se, Cu2Te, Cu4GeS4, Cu2SnS3, Cu2SnSe3, GeS2, GeSe2, Ge4Se9, Sb2S3, Sb2Se3, Sb2Te3, SnS and SnSe are presented. Two density functional theory based on methods are used, the Vienna Ab initio Simulation Package (VASP) and the orthogonalized linear combination of atomic orbital (OLCAO) method. In particular, the concept of total bond order density (TBOD), a single quantum mechanical metric characterizing the internal cohesion of a crystal is used to compare and correlate with the calculated results on the physical properties of these crystals. These detailed calculations of a large sample of chalcogenide crystals, using the same computational methods enable us to draw insightful conclusions for the first time on the general principles governing the specific properties of chalcogenide crystals and glasses.