For calculations, two fairly simple clusters were taken: Zn_4S_4 for sphalerite and Zn_6S_6 for wurtzite. The results of calculations of bond lengths and a number of energy characteristics for less complex clusters of sulfide minerals are presented in table 1, figures 1 and 2 show geometric models of two simple clusters of sphalerite and wurtzite.

Table 1 – Geometric, electronic characteristics and enthalpy of formation of sphalerite and wurtzite clusters

Compound, composing elements	q, units of charge	r, nm	$\Delta_f H$, kJ/mol	Ionization potential, eV	μ, D	E_{HOMO}, eV	E_{LUMO}, eV
Sphalerite S Zn Zn - S	 -0,001 +0,001	 0,24	-1244,36	11,04	0	-11,04	-3,08
Wurtzite S Zn Zn – S	 -0,12 +0,12	 0,23	-2112,13	10,36	0,001	-10,36	-5,04

Table 1 shows that in the model clusters of sphalerite and wurtzite, the Zn-S bond length is 0.241 nm and 0.231 nm, respectively. The latter shows that an increase in the number of atoms in the model cluster leads to a certain reduction in the length of the Zn-S bond.

In all the models studied, the positive charge is concentrated on the metal atoms, and the negative charge on the sulfur atoms. The electron density in all clusters is higher for the more electronegative sulfur atom.

All clusters taken for study are thermodynamically stable, since they are characterized by negative values of enthalpy of formation. The enthalpy of formation, in addition, is the energy characteristic of bonds in clusters. Proceeding from this, a comparison of this characteristic for clusters of the same type of zinc sulfides indicates a large thermodynamic stability of the wurtzite cluster.

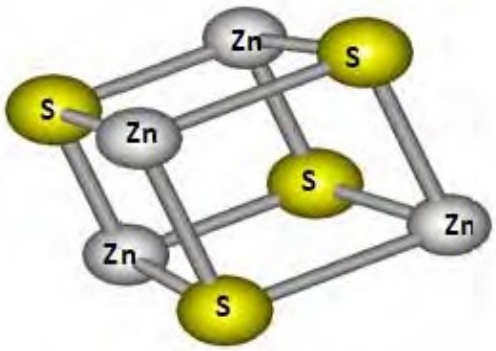

Figure 1 – Geometric model of sphalerite cluster Zn_4S_4

Figure 2 – Geometric model of the wurtzite cluster Zn_6S_6