Ab initio investigations of double rare earth fluorides under pressure

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There is a considerable progress in the study of structural and mechanical properties pressure effect in $M\mathrm{LiF_4}$ (M — is an element belonging to the group of lanthanides) compounds. The study of $M\mathrm{LiF_4}$ systematics behavior under compression may lead to deeper understanding of phase transitions mechanisms of named materials. For example, Grzechnik et al. studied $\mathrm{GdLiF_4}$ [1], $\mathrm{YLiF_4}$ [2] and $\mathrm{LuLiF_4}$ [3] compounds by X-ray diffraction in a diamond anvil cell at room temperature under pressure. These three compounds modifications took place near the pressure of 11 GPa with different consequences.

For investigation of applied pressure influence on $\mathrm{GdLiF_4}$ and $\mathrm{LuLiF_4}$ properties (structural, mechanical, electronic and vibrational) density functional theory (DFT) was used [4,5]. Ab initio calculations were performed using *Vienna Ab Initio Simulation Package* VASP 5.2 module [6] of MedeA® software package (Materials Design, S.A.R.L.). As a result of pressure influence investigation $\mathrm{GdLiF_4}$ structural decay reasons were determined. Also $\mathrm{LuLiF_4}$ second-order phase transition was proved and its direction in the $(\mathrm{LuLiF_4})_4$ unit cell was found. Coefficient at quadratic order parameter was calculated and its dependence on the pressure has been plotted indicating a phase transition at 10.5 GPa. Absence of phase transitions in the structures with symmetries $\mathrm{P2_1/c}$ and P12/c1 of $\mathrm{LuLiF_4}$ compound were proved by comparison of the enthalpy of these phases with the enthalpy of scheelite phase $\mathrm{I4_1/a}$.

References

[1] Decomposition of $\mathrm{LiGdF_4}$ scheelite at high pressures/A. Grzechnik, W.A. Crichton, P. Bouvier [et al.]//Journal of Physics: Condensed Matter. – 2004. – V. 16, no. 43. – P.7779.

[2] Scheelite to fergusonite phase transition in $\mathrm{YLiF_4}$ at high pressures/A. Grzechnik, K. Syassen, I. Loa [et al.]//Phys. Rev. B. – 2002. – V.65, no. 10. – 104102.

[3] Pressure-induced tricritical phase transition from the scheelite structure to the fergusonite structure in $\mathrm{LiLuF_4}$/A. Grzechnik, K. Friese, V. Dmitriev [et al.]//Journal of Physics: Condensed Matter. – 2005. – V.17, no. 4. – P.763.

[4] Hohenberg, P. Density functional theory/P. Hohenberg, W. Kohn//Phys. Rev. B. – 1964.– V.136. –Pp. 864-876.

[5] Kohn, W. Self-consistent equations including exchange and correlation effects/W. Kohn, L.J. Sham//Phys. Rev. A. – 1965. – V. 140, no. 4A. – P.A1133.

[6] Kresse, G. Efficient iterative schemes for ab initio total-energy calculations using a plane-wave basis set/G. Kresse, J. Furthmuller//Phys. Rev. B. – 1996. –V.54, no.16. – P.11169.