Crystal-structure prediction and experimental investigation of the polymorphic lanthanum fluoride selenides LaFSe and La_2F_4Se

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Supporting Information

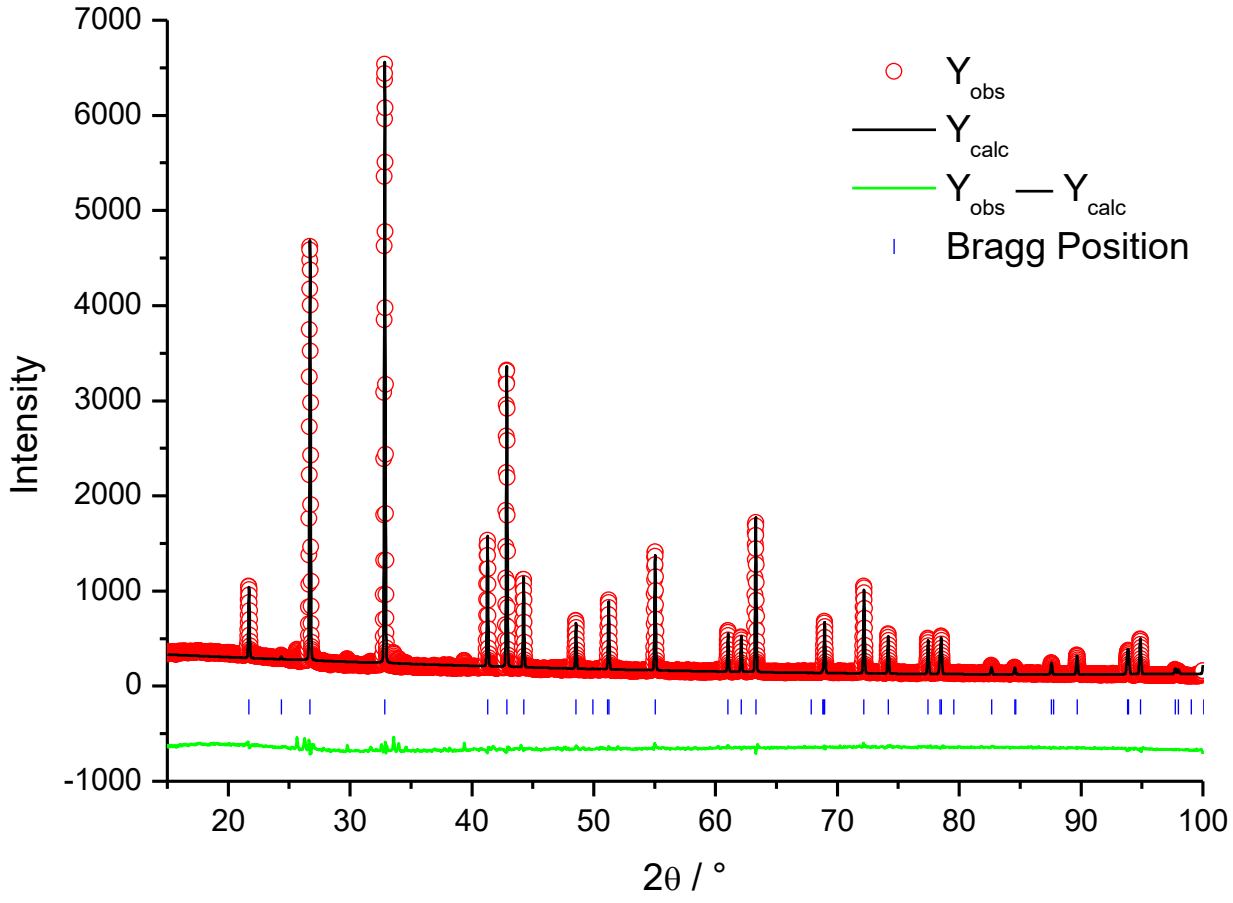

Figure S1. Powder X-ray diffraction pattern for the structure refinement of the B-type LaFSe modification in the 2Θ-range between 15 and 100 ° using Cu-K_α radiation.

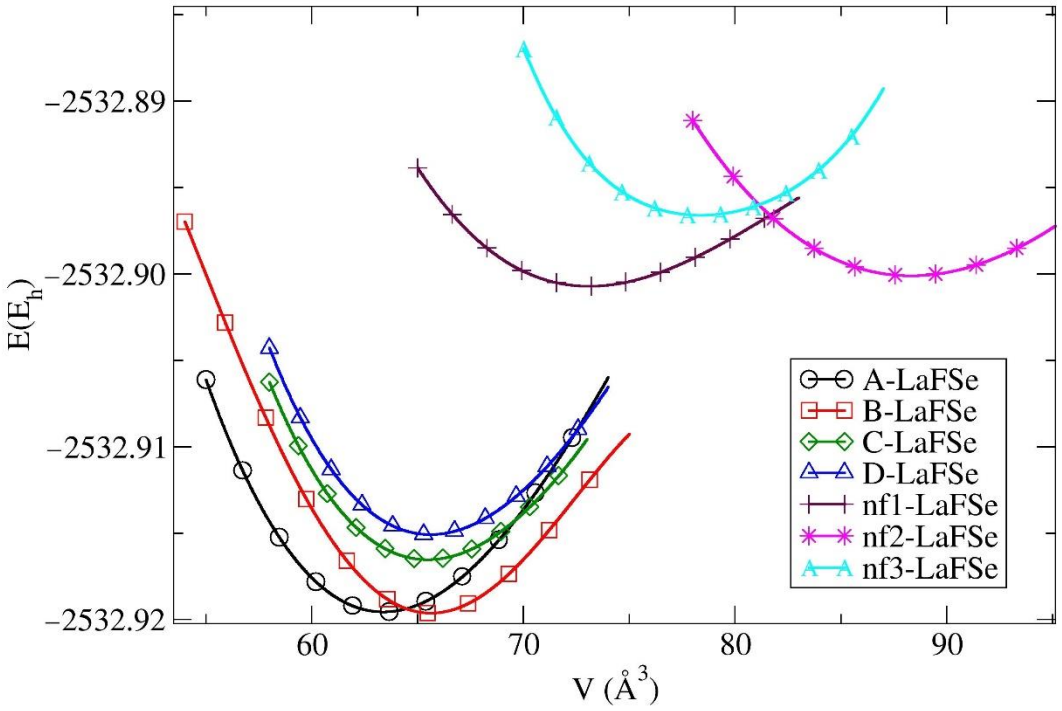

Figure S2. Energy vs. volume curves, E(V), for the most relevant structure candidates computed in the LaFSe system using the GGA-PBE functional. Energies per formula unit are given in Hartree (Eh).

Modification	LDA	GGA	B3LYP	HSE06
***A*-LaFSe**	−2529.2172	−2532.8609	−2533.1257	−2532.9196
***B*-LaFSe**	−2529.2165	−2532.8620	−2533.1251	−2532.9195
***C*-LaFSe**	−2529.2141	−2532.8581	−2533.1220	−2532.9161
***D*-LaFSe**	−2529.2127	−2532.8565	−2533.1205	−2532.9145
***nf1*-LaFSe**	−2529.1945	−2532.8438	−2533.1100	−2532.9007
***nf2*-LaFSe**	−2529.1842	−2532.8443	−2533.1160	−2532.9004
***nf3*-LaFSe**	−2529.1879	−2532.8412	−2533.1103	−2532.8969

Table S1. Ground state energies of the seven most promising structures and structure candidates in the LaFSe system.