Supporting Information

In the calculation, there are two important parameters: cut-off energy and exchange correlation functional. Choosing the appropriate cut-off energy and exchange correlation functional is the key to making the calculated value close to the experimental value.

When the fixed cut-off energy was 300 eV, different exchange correlation functions were employed for calculation, and the results are shown in Table 1. It can be seen from Table 1 that when the cut-off energy is 300 eV, the deviation of unit cell parameters calculated under the exchange correlation functional GGA-PBESOL is minimal from the experiment values. Therefore, GGA-PBESOL is selected as the exchange correlation functional.

Table 1. The unit cell parameters of fluorite under different exchange correlation functional.

Computation Function	Lattice Parameter/Å	Deviation/%
LDA-CA-PZ	5.385	–0.0143
GGA-PBE	5.569	0.0195
GGA-RPBE	5.681	0.0399
GGA-PW91	5.567	0.0190
GGA-WC	5.485	0.0040
GGA-PBESOL	5.481	0.0034

Note: the deviation representing deviations of calculated values from reference values (5.4631 Å), the same as follows.

Under exchange function GGA-PBESOL, different cut-off energies of plane wave was selected for the optimizing calculation of fluorite cell model, and the calculation results are shown in Table 2. From Table 2, when the cut-off energy reaches 330 eV, the deviation reaches the minimum value. Then with the increase of cut-off energy, the deviation is further expanded. In order to minimize the calculation deviation, the calculated cut-off energy is 330 eV.

Table 2. The unit cell parameters of fluorite under different cut-off energy.

Cut-off Energy/eV	Lattice Parameter /Å	Deviation/%
270	5.570	0.0195
300	5.482	0.0034
330	5.448	−0.0028
370	5.434	−0.0054
400	5.429	−0.0063