International Journal of Applied
and Natural Sciences (IJANS)
ISSN(P): 2319-4014; ISSN(E): 2319-4022
Vol. 8, Issue 3, Apr - May 2019; 109-116


International Academy of Science,
Engineering and Technology
Connecting Researchers; Nurturing Innovations

# ENERGY PARAMETERS OF INTRACELLULAR MOVEMENT OF FLUORIDE IONS IN A SUPERIONIC $LaF_3$ NANOCRYSTAL

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## *ABSTRACT*

*The paper presents the results of quantum chemical calculations of the change in the lattice energy and the energy parameters of internal motion in a $LaF_3$ nanocrystal during a phase transition from a dielectric state to a highly conducting phase. Quantum-chemical calculations were done for three nanogrids with linear dimensions of 2.1 × 2.0 × 2.2 nm, 2.9 × 2.0 × 2.2 nm and 3.5 × 2.0 × 2.2 nm. It has been established that the increment in the magnitude of the lattice energy in all nanolattices decreases with an increase in the number of disordered fluorine ions in them. It was also established that the increment of the lattice energy (with an equal number of disordered fluorine ions) is more significant for nanogrids with a larger number of ions. It is shown that, for all nanogratings, the energy $E_a$ of a single act of disordering of the anion sublattice with an increasing number of disordered ions decreases from 0.16–0.17 eV in the dielectric phase to 0.02–0.04 eV in the superionic state.*

***KEYWORDS:*** *Quantum Chemical Calculation, $LaF_3$ Nanocrystal, Internal Motion*

***Article History***

***Received:*** *17 Apr 2019* **|** ***Revised:*** *26 Apr 2019* **|** ***Accepted:*** *07 Apr 2019*