

## Pairs of Ln(III) dopant ions in crystalline solid luminophores : an *ab initio* computational study.

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### Rok wydania

2016

### Czasopismo

Journal of Rare Earths

### Numer woluminu

34

### Strony

820-827

### DOI

10.1016/S1002-  
0721(16)60100-X

### Kolekcja

Naukowa

### Język

Angielski

### Typ publikacji

Artykuł

### Streszczenie

Formation of dopant ions clusters in solid (glass) luminophores may affect efficiency of non-radiative energy transfer processes between dopant (photoactivator) ions via shortening of the effective distance between them. This study was based on the assumption that the distance between the dopant ions affects the energy of crystal volume at proximity. According to this idea, semi-empirical and *ab initio* density functional theory (DFT) calculations were performed on various supercells of YVO<sub>4</sub>:Eu<sup>3+</sup> as a model system. It was noted that a shorter Eu–Eu distance resulted in lower total energy of the system, compared to an analogous structure with distant Eu<sup>3+</sup> ions. As lower energy configurations are preferred, the observed phenomenon was considered to be related to dopant ions clusters formation. Additionally, the values of energies obtained from DFT calculations were used to estimate the percentage of dopant ions occurring as pairs, for different dopant concentrations. The estimation agreed quite well with the available literature data.

### Słowa kluczowe

crystalline, luminophore, lanthanides, vanadate, dopant clustering, rare earths, density functional theory

### Adres publiczny

[http://dx.doi.org/10.1016/S1002-0721\(16\)60100-X](http://dx.doi.org/10.1016/S1002-0721(16)60100-X)

### Strona internetowa wydawcy

<http://www.elsevier.com>