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Ab Initio Calculations of the Structural and Dynamical Properties of Copper Pyrophosphate †

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Abstract: In our research, we apply the density functional theory and lattice dynamics calculations to get a better insight into the structural and dynamic properties of the $Cu_2P_2O_7$ crystal. All calculations were performed with the Vienna Ab initio Simulation Package (VASP) within the general gradient approximation (GGA). The obtained results were compared with the experimental measurements of nanocrystalline copper pyrophosphates.

Keywords: pyrophosphate; ab initio; numerical calculations; Raman scattering

1. Introduction

Pyrophosphate nanocomposite materials containing transition metal ions have unique physical, chemical, electrical and mechanical properties [1]. Especially interesting characteristics show compounds containing cooper atoms, which have received a lot of attention in research and application due to its excellent conductivity as well as good biocompatibility. The study of copper pyrophosphate compounds is a subject of increasing interest because of their enhanced electrical and photonic properties as well as materials science applications [2].

2. Discussion

The elementary cell of a nanocrystalline copper pyrophosphate was reproduced on the base of experimental data on lattice parameters and atomic positions. Then we made optimization of the crystal structure with the VASP software [3] using the density functional theory (DFT) and DFT + U calculation methods. We performed calculation of the electronic density of states considering the ferromagnetic (FM) and antiferromagnetic (AFM) spin order. The optimized crystal structure have been compared with the experimental data. The phonon dispersion curves and density of states were calculated using the Phonon program [4].

The obtained results of numerical calculations revealed better consistency of structural parameters with the experimental data for the AFM order. The value of the magnetic moment on the copper atom amounts to 0.84 μ_B and the resulted value of the energy band gap for the optimized structure is equal to 2.85 eV. The phonon spectra show a good agreement with the experimental Raman. Obtained results confirm that copper pyrophosphate could have a numerous applications especially in the fields of magnetism and nanophotonics.

References

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