THEORETICAL MODELLING OF THE LUMINESCENCE SPECTRA OF OXIDE CRYSTALS AWO_4 (A=Zn, Pb) WITH DEFECTS

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Oxide crystals AWO_4 (A=Zn, Pb) are considered as a promising scintillations material for various purposes in the high energy physics and technological applications.

Recently we developed a cluster approach for theoretical investigation of the electronic structure of oxide crystals based on the configuration interaction (CI) computation with account for changes of atomic coordinates which modelled lattice vibrations [1-3]. The electronic structures of luminescence centers AWO_4 crystals are calculated using embedded cluster approach. Clusters considered for calculations consisted of two regions: ab-initio region which comprised atoms of possible luminescence centers (one tungstate group WO_6^{6-} and the closest to it A^{2+} (A=Zn, Pb) cation and the region of effective potentials which included several thousands of surrounding atoms treated in calculations as point charges. The energies of electronic states and oscillator strengths of electronic transitions in the ab-initio regions are obtained in computation based on Configuration Interaction (CI) approximation using GAMESS program package [4]. The crystals with both regular structure and with point defects (oxygen vacancy V_O and molybdenum impurity) were modelled in the ab-initio regions.

Dependencies of the electronic energies of luminescence centres in these crystals on changes of atomic coordinates which modelled lattice vibrations are calculated. Vibrations of WO_6^{6-} groups in AWO_4 (A=Zn, Pb) crystals were modelled in calculations via considering the displacements of the nuclear positions in the ab-initio region. Luminescence emission and excitation spectra of AWO_4 (A=Zn, Pb) crystals were constructed using the obtained configuration curves, and these spectra were compared with corresponding experimental data. Discrepancies between experiment and calculations are discussed.

References:

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