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Theoretical modelling of luminescence processes in oxide glass-ceramic nanocomposite materials

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The optical properties of glass-ceramic nanocomposite materials "oxide-glass matrix @ oxide-crystalline micro/nanoparticles filler"are now the subject of intensive research. The unique physical properties of such composites are determined by interphases regions, which have atomic structure and chemical composition intermediate between the crystalline and glass components. The atomic structure of interphases can be obtained in calculations by molecular dynamics (MD) methods. Further application of the electronic structure calculations allows to obtain the most important micro- and macro-characteristics of the interphase layers and thus to explain the experimentally observed properties of glass-ceramic composites.
This report presents results of complex computational and experimental studies of the atomic and electronic structures of luminescent oxide glass-ceramic composite materials. Three different types of glass-ceramic composited are considered: a) KBi(MoO4)2 crystal @ K2O-P2O5-MoO3-Bi2O3 glass b) K2Bi(PO4)(WO4) crystal @ K2O-P2O5-WO3-V2O5 glass; c) LaVO4 crystal @ Li2O-V2O5-B2O3 glass. The atomic structures of interphase regions were calculated by MD methods. The electronic structure calculations were performed in the DFT approximation using the band-periodic plane wave pseudopotential method. The excited electronic states and optical spectra of possible centers of luminescence of glass-ceramic composite materials are calculated using the Time-Dependent Density Functional Theory (TD-DFT) within molecular cluster approach.
Obtained computational results are compared with experimental data on structural analysis, optical and luminescence spectroscopy. The mechanisms of luminescence and excitation energy transfer in oxide glass-ceramics of different types are discussed.

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Presence at Taras Shevchenko National University

Primary author: Dr HIZHNYI, Yuriy (Taras Shevchenko National University of Kyiv)

Co-authors: Prof. NEDILKO, Serhii (Taras Shevchenko National University of Kyiv); BORYSIUK, Viktor (Taras Shevchenko National University of Kyiv); Dr CHORNII, Vitalii (National University of Life and Environmental Sciences of Ukraine); ZHYDACHEVSKYY, Yaroslav (Institute of Physics, Polish Academy of Sciences)

Presenter: Dr HIZHNYI, Yuriy (Taras Shevchenko National University of Kyiv)

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