# ELECTRONIC STRUCTURE, OPTICAL PROPERTIES AND MECHANISMS OF LUMINESCENCE OF $Zn(MoO_4)$, $NaAl(MoO_4)$ AND $Li_2Zn_2(MoO_4)_3$ MOLYBDATE CRYSTALS

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Molybdate compounds with light cations are considered as perspective materials for novel scintillator applications [1, 2] as well as promising laser host matrixes [3]. The work presents results of experimental studies of the luminescence properties and theoretical calculations of the electronic structure and optical constants of the set of molybdate crystals perspective for various scientific and technical applications.

Photoluminescence (PL) and PL excitation spectra of the synthesized molybdates were studied at 4.2, 77 and 300 K with use of xenon lamp and various laser sources generating in visible spectral region. The VUV-excited time-resolved luminescence spectra were obtained on SUPERLUMI station at HASYLAB (DESY), Hamburg, Germany in 4 – 16 eV excitation energy region. Electronic structures of perfect $Zn(MoO_4)$, $NaAl(MoO_4)$, $Li_2Zn_2(MoO_4)_3$ and $NaAl(MoO_4)$ with $Cr^{3+}$ impurities, were calculated by the full-potential linear-augmented-plane-wave (FLAPW) method [4]. Structures of one-electron bands, energy dependencies of the components of dielectric tensor, reflection and absorption spectra were calculated.

The origin of the luminescence centers is discussed. Features of the reflectivity and luminescence excitation spectra and peculiarities of energy transfer to the luminescence centers are explained using the calculated partial densities of electronic states and optical constants. Dependencies of the PL emission and excitation spectra of $NaAl(MoO_4)_2$:$Cr^{3+}$ crystals on temperature and $Cr^{3+}$ concentration are analyzed. The origin of the VUV excitation bands of $NaAl(MoO_4)_2$:Cr crystals is ascertained.

References

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