LUMINESCENT PROPERTIES AND ELECTRONIC STRUCTURE OF THE MOLYBDATES WITH LITHIUM AND ZINC CATIONS

V.V. Mikhailin[1,2], D.A. Spassky[1], A.N. Vasil'ev[1], I.A. Kamenskikh[2], V.N. Kolobanov[2], A.E. Savon[2], L.Yu., Berezovskaya[3], L.I. Ivleva[3], I.S. Voronina[3], Yu.A. Hizhnyi[4], S.G. Nedilko[4], O.P. Barinova[5], S.V. Kirsanova[5], A.A.Pavlyuk[6], S.F.Solodovnikov[6], Z.A.Solodovnikova[6], E.S.Zolotova[6]

[1]Skobeltsyn Institute of Nuclear Physics, Moscow State University, 119991, Moscow, Russia
[2]Physics Faculty, Moscow State University, 119991 Moscow, Russia
[3]A.M. Prokhorov General Physics Institute of RAS, Vavilov str. 38, 119991, Moscow, Russia
[4]Kyiv National Taras Shevchenko University, Hlushkova ave. 2, bl. 1, 03680 Kyiv, Ukraine
[5]D. Mendeleyev University of Chemical Technology of Russia, 125047, Moscow, Russia
[6]Nikolaev Institute of Inorganic Chemistry, 630090 Novosibirsk, Russia

E-mail: deris2002@mail.ru

Recently molybdates attracted attention as novel materials for the cryogenic phonon – scintillating detectors (Mikhailik and Kraus, 2006; Pirro et al., 2006, Barinova et al, 2008). Simultaneous registration of the scintillation and phonon signals allows to reduce background and makes it suitable to search for neutrinoless double beta decay and dark matter. Molybdate single crystals are considered as a material for cryogenic detectors due to the rather high light yield at the low temperatures and presence of molybdenum isotope ^{100}Mo that is one of the most promising double beta decay candidate. Absence of the long-lived radioactive isotopes in lithium and zinc is an important advantage that allows to reach a low level of radioactive background required by the double beta and dark matter experiments. Here we present the results of the luminescent properties investigation and electronic structure calculations for Li_2MoO_4, $Li_2Zn_2(MoO_4)_3$ and $ZnMoO_4$ single crystals. Luminescence of these compounds is almost unexplored. The origin of the luminescence centers is discussed in the presentation. To our knowledge no electronic structure calculations for the molybdates with lithium and zinc cations were performed so far. The features of the reflectivity and luminescence excitation spectra and peculiarities of the energy transfer to the luminescence centers are also discussed in the presentation using the calculated partial densities of electronic states and optical constants.

Luminescence, thermo-stimulated luminescence, excitation and reflectivity spectra were measured at the Superlumi station (DESY, Hamburg) and at the laboratory set-up as well. Electronic structure of the perfect molybdate crystals were calculated by the full-potential linear-augmented-plane-wave (FLAPW) method (Blaha et al., 2001).

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