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ELECTRONIC STRUCTURE AND OPTICAL PROPERTIES OF Li2MoO4 AND ZnMoO4 CRYSTALS

The set of lithium molybdates Li2MoO4 crystals were made by the Czochralski (CZ) technique at different growing conditions. The electronic band structures of ZnMoO4 and Li2MoO4 crystals were calculated by the Full-Potential Linear Augmented Plane Wave (FLAPW) method. Transmittance spectra of Li2MoO4 crystals reveal additional absorption bands near 370 nm. Calculations revealed different contributions from the cationic states (Li and Zn) to the electronic Conduction band of Li2MoO4 and ZnMoO4 crystals, respectively.

Primary authors: HIZHNYI, Yuriy; NEDILKO, Serhii (Taras Shevchenko National University of Kyiv); Dr CHORNII, Vitalii (Taras Shevchenko National University of Kyiv); BORYSIUK, Viktor (Taras Shevchenko National University of Kyiv, Faculty of Physics, Chair of Optics)

Presenter: HIZHNYI, Yuriy

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