

Electronic Band Structures of LiGaO₂ under Pressure: First Principles Study

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Beside the natural phase, LiGaO₂ under different pressure conditions can be stable in different structures [<http://dx.doi.org/10.1016/j.ceramint.2017.05.247>]. The structures of LiGaO₂ were named WZ', HX', BCT', RS' and RS'' in analogous with the well-known phases of ZnO. In this work, the electronic band structures of those phases were studied. We found that the bandgap as well as the bandgap type (direct/indirect) are strongly depend on the crystal structure. In addition, for selected crystal structures, the changes of the band gaps with respect to the pressure, i.e., the bandgap deformation potentials, were studied. Our results illustrated that the bandgap of LiGaO₂ can be modified by applying pressure in different conditions. The details of the electronic band structures for different phases of LiGaO₂ and the pressure dependence of selected phases will be presented and discussed.

Primary author: Dr SAILUAM, Wutthigrai (Rajamangala University of Technology of Technology Khon Kaen Campus)

Co-authors: Dr PHACHEERAK, Kanoknan (College of Nanotechnology, King Mongkut's Institute of Technology); Prof. LIMPIJUMNONG, Sukit (School of Physics and NANOTEC-SUT Center of Excellence on Advanced Functional Nanomaterials, Suranaree University of Technology)

Presenter: Dr SAILUAM, Wutthigrai (Rajamangala University of Technology of Technology Khon Kaen Campus)

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