# Geodynamics Seminar

## 第309回ジオダイナミクスセミナー

# Pressure and compositional dependence of the lattice dynamics of $LiGaO_2$ investigated by Raman scattering experiments and ab initio calculations

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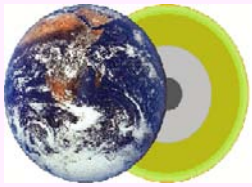
主催：愛媛大学地球深部ダイナミクス研究センター
日時：11/18（金）午後 4時30分～
場所：総合研究棟 4F 会議室



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## Abstract

The effects of pressure on vibrational properties of orthorhombic, hexagonal, and cubic phases of $LiGaO_2$ have been studied by means of high-pressure Raman scattering spectroscopy and *ab initio* calculations. The orthorhombic and hexagonal phases were evidenced to undergo irreversible phase transitions at ~14 and ~25 GPa, respectively. Pressure dependence of Raman phonon frequencies for these three polymorphs of $LiGaO_2$ has been studied. The pressure coefficients and mode Grüneisen parameters for their Raman phonon modes are reported. By comparing pressure dependence of Raman phonon behavior between cation-ordered hexagonal phase and cation-disorder cubic phase, the effect of substitional disorder on lattice anharmonicity has been evaluated. The obtained structural parameters and vibrational properties are compared and discussed to the results of our *ab initio* calculation.

詳細は当センターホームページ: http://www.ehime-u.ac.jp/~grc/をご覧ください
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