博士論文公聴会の公示（物理学専攻）

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論文題目：Electronic band structures and optical properties of $LiCaAlF_6$ and $LiYF_4$ crystals as potential vacuum ultraviolet materials in equilibrium and high pressure conditions

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論文要旨:

The electronic band structures and optical properties of perfect lithium calcium hexafluoroaluminate (LiCaAlF6, LiCAF) and lithium yttrium tetrafluoride (LiYF4, LiYF) crystals have been studied numerically and experimentally as potential vacuum ultraviolet (VUV) materials. Using optimized unit crystal volumes and equilibrium lattice constants, I found LiCAF and LiYF have an indirect band gap of 12.23 eV and a direct band gap of 11.09 eV, respectively. I also predicted how the band gap energies will shift upward with the application of high pressure through uniform volume and uniaxial compressions. At a pressure of 110.10 GPa applied through uniform volume compression, the band gap of LiCAF shifts from an indirect band gap of 12.23 eV at equilibrium (0 GPa) to a direct band gap of 14.21 eV. On the other hand, LiYF crystal maintains its direct band gap of 11.87 eV under high pressure up to 50 GPa. The uniform and uniaxial compressions under high pressure are investigated not only to modify the band gap energy but also to find out the best conditions to obtain the maximum direct band gap for these two fluorides. Based on the theoretical and experimental results, it is more effective to apply pressure along the c-axis in order to increase the LiCAF and LiYF band gap energies. The optical properties such as refractive index, extinction coefficient, absorption coefficient, and reflectivity are also investigated at different pressures based on the real and imaginary parts of the dielectric function.

With these results, this study will lead not only to the better understanding of the fundamental physical phenomena and underlying mechanisms involving wide band gap fluoride crystals but also to the development of new optical devices in the VUV region. High pressure compression can also be applied to other fluoride crystals to improve their properties toward VUV applications.