

# 연구 발표 초록

초청강연(Plenary Lecture)

(PL-1)

## 층상구조화합물의 전자상태계산 Electronic Structure and Chemical Bonding of Layered Structure

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The purposed of this study is to contribute to the subjects of (1) constructing the electronic structure and chemical bonding of the host materials, and (2) entering into the detailed description of the intercalate complex. This study is especially focus on the charge state of Li and the magnitude of covalency around a Li atom when it intercalates the hosts and how the chemical bondings in various layered compound are modified by the Li-intercalation. In this investigation, we calculated the electronic structure of layered compound using DV-X $\alpha$  molecular orbital method<sup>1)</sup>.

참고문헌)

1. 처음배우는 전자상태계산., 도서출판 한림원
2. 양자재료학의 기초., 도서출판 한림원

1) <http://www.dvxa.net> --> research ---> 연구용계시판에서 프로그램 공짜로 다운로드가능