

리튬 이차 전지로의 응용을 위한 LiNiO_2 양극 물질의 전자 상태 연구
Electronic state of LiNiO_2 cathode materials for Li ion barriers

전영아, 김양수, 노광수
한국과학기술원
(yajeon@kaist.ac.kr)

The layered nickel oxides (LiNiO_2) have been studied for possible use as cathode materials in 4V lithium batteries. Although LiCoO_2 has been known as the best candidate material for Li-ion batteries, which produces the best performance LiNiO_2 is generally accepted as an attractive cathode material, because of its various advantages such as lower cost, higher discharge capacity and better reversibility. In this investigation, we calculated the electric state of LiNiO_2 using DV-X α molecular orbital method in order to obtain the information of chemical bonding among the Li, Ni and O. In LiNiO_2 , alternate layers of Li and Ni occupy the octahedral sites of a cubic close packing of oxide ions, making up a rhombohedral structure with an R-3m space group, Li in 3a, Ni in 3b, and O in 6c sites. On the basis of this, we made the cluster model and studied ionization of each atoms and interaction between atoms according to Mulliken population analysis.