

## [II~6]

The electronic and magnetic properties of 3d transition-metal impurities in aluminum.

ByungSub Kang, HaengKi Lee, MyoungJin Lee, SuckWhan Kim(Andong Univ.), KiSoo Sohn(Kyungpook Univ.)

Dept. of physics, Kyungpook National University.

Abstract : First-principles electronic structure calculations were performed for a  $Al_{55}$  and  $Al_{54}M$  embedded clusters, where M stands for Fe, Co and Ni. At the equilibrium positions of the Al first neighbors around Fe, Co and Ni, obtained by total energy minimization, it was found that the local moment of the impurities and the spin polarization of the Al atoms surrounding the impurities in all cases. The result is consistent with the experiment and the other calculations, and renders unnecessary a microscopic description based on spin fluctuations.