Electronic and magnetic properties of cathode materials for Li-ion batteries studied by electronic structure calculations

M. Rybski,[1] J. Molenda,[1] and J. Tobola[1]

[1] *AGH University of Science and Technology, Krakow, Poland*

The close correlations between electronic structure and electrochemical properties of lithium-ion cathode materials have been investigated in recent years. In particular, the impact of electronic structure features on the discharge curve in A_xMO_2 (A=Li, Na, M=Mn, Co, Ni) has recently been reported based on experimental and theoretical investigations [1,2]. We present results of electronic structure calculations for a novel variant of the well-known Li-ion battery material $Li_xCo_{1-y-z}Ni_yMn_zO_2$, using the Korringa-Kohn-Rostoker method with the coherent potential approximation, which is especially well adapted to account for complex chemical disorder. Electronic densities of states computed for different Li and Co/Ni/Mn concentrations show that electronic structure of $Li_xCo_{1-y-z}Ni_yMn_zO_2$ exhibits half-metallic properties in wide range of Li content. Noteworthy, magnetic moments of Co, Ni and Mn can be a subject of magnetic frustration due to the rhombohedral crystal structure. It is found that computed density of states details are sensitive to assumed magnetic ordering and also to deformation of O octahedra.

References:

[1] J. Molenda *et al.*, Physical Chemistry Chemical Physics, **16** (2014) 14845.
[2] A. Milewska *et al.*, Solid State Ionics, **263** (2014) 110–118.