

***Ab initio* Materials Design for TCO-based New-functional Materials**

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Based upon *ab initio* electronic structure calculations for delafossite CuAlO_2 and wz ZnO , we report materials design for TCO-based new-functional materials, such as (i) low-resistive *p*-type ZnO and CuAlO_2 by co-doping, (ii) high-efficient thermoelectric power in CuAlO_2 ($ZT > 3$) by *p*-type doping, (iii) half-metallic ferromagnetism in transition-metal-impurity doped CuAlO_2 and ZnO -based diluted magnetic semiconductors (DMS), and (iv) quasi-one-dimensional nano-magnet with high Curie temperatures (T_c) caused by two-dimensional nano-scale spinodal decomposition by layer-by-layer crystal growth in MBE or MOCVD.

We propose that oxygen interstitial acceptor and Cu-vacancy is the most promising candidate for the realization of *p*-type CuAlO_2 . We also propose the Ga (or Al or In) and N-codoping works very well for the fabrication of low-resistive *p*-type ZnO . We have designed that the half-metallic and high-spin ferromagnetic state is expected to be stable in Mn-, Fe-, Co- and Ni-doped transparent delafossite CuAlO_2 .

We propose materials design of ferromagnetic CaO, SrO, BaO, MgO, and SiO_2 without any transition metal elements based on first principles calculations. It is found that in C or N-doped CaO, SrO, BaO, MgO and N-doped SiO_2 the ferromagnetic states could be stable.

We show that spinodal decomposition under the layer-by-layer crystal growth condition leads to characteristic quasi-one-dimensional nano-structures in DMS. It is found that the DMS systems can form rather large clusters with highly anisotropic shape even for low concentrations. It is suggested that the blocking phenomena in the superparamagnetism, the magnetic dipole-dipole interaction and the network of the one-dimensional structures should be considered to understand the magnetism in DMS.

Based on *ab initio* calculations of chemical pair-interactions of magnetic impurities in DMS and on Monte Carlo simulation of the layer-by-layer crystal growth, we design a new fabrication process in the bottom-up nanotechnology to realize the Tera-bit-density nano-magnets by controlling the self-organized two-dimensional spinodal decomposition. We show that the growth position, shape and density of quasi-one-dimensional nano-magnets in the DMS can be controlled by the nano-scale seeding and the vapor pressure or concentration of the doped magnetic-impurities under the thermal non-equilibrium crystal-growth condition in MBE, MOVPE or MOCVD.

We also discuss the difference in the electronic structure between the LDA and the self-interaction corrected LDA (SIC-LDA) by comparing with the photoemission experiment, if time is available. We have developed our material design method to include self-interaction correction (SIC) to the local density approximation. We employed the pseudo-SIC method proposed, and implemented the method into the KKR-CPA-LDA package. We applied the method to DMS systems and calculated electronic structure, magnetic interactions and Curie temperatures of ZnO .

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