Information on Doctoral Thesis of Fellows Pham The Tan

Official thesis title: ***Structure and properties of single and double perovskite manganites***

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3. Date of birth: 17th September, 1980

4. Place of birth: Hai Duong - Viet Nam

5. Admission decision number: Decision No. 2385/QĐ- SĐH dated 29th June 2007 of the President of Vietnam National University, Hanoi.

6. Changes in academic process: None

7. Official thesis title: ***Structure and properties of single and double perovskite manganites***

8. Major: Physics.

9. Code: 62440104.

10. Supervisors: Assoc. Prof. Hoang Nam Nhat, VNU University of Engineering and Technology.

11. Summary of the new findings of the thesis

- We have successfully fabricated the single and double perovskite manganites $CaFe_xMn_{1-x}O_3$ (x = 0; 0,01; 0,03; 0,05) and $La_2Co_{1-x}Fe_xMnO_6$ (x = 0; 0,01; 0,02; 0,03). We studied their structures and properties by means of highly precise experimental techniques such as the X-Ray diffraction, Raman scattering, IR-absorption, resistivity measurements, magnetic susceptibility measurements … The results of our research were published in 10 publications in the scientific journals in the field of the research.

- By means of the modeling methods we studied all possible magnetic configurations for $CaMnO_3$ and showed that the ferromagnetic configuration might prevail in the nanometer scale. All these magnetic configurations can practically exist, providing that the conditions satisfy, and there are the structural deformations so that the ferromagnetic interactions can prevail and lead to the ferromagnetism. The appearance of ferromagnetism in ceramic compounds is the topic of interests for decades. The optimized values for G-AF ground state in $CaMnO_3$ are: E_g = 1,09 eV, Δ_{pd} = 3 eV and U = 6,2 eV; for the thin films the ground state should be the insulating C-AF. The energy gap between G-AF and C-AF states in the bulk samples should be around 16 meV, that induces the T_C about 185 K. At the size less than 2,7 nm the penetration of ferromagnetism into the inside layers may reach 3,5 layers and induce the ferromagnetism. The band-gaps for the thin films are smaller than that of the bulks.

- In the single-layer perovskite system $CaFe_xMn_{1-x}O_3$ (x = 0.01, 0.03, 0.05), the replacement of Mn by Fe forced the decrease of magnetization, but the similar replacement in the double perovskite manganites

$La_2Co_{1-x}Fe_xMnO_6$ induced the increase of saturated magnetization besides the decrease of T_C and coersive-field strength H_c. The resistivity of the samples was also decreased but the conduction mechanism remained unchanged and the Variable-Range-Hopping (VRH) model was still considered as the most probable. The decrease of ferromagnetic interaction from 3D to 2D (i.e. from $CaMnO_3$ to $La_2CoFeMnO_6$) also induced the decrease of the magnetization and coercive-field strength. The dependence of T_C on doping level also agreed well with the empirical models and with our modified rule. The influence of Fe- concentration on the ratio Mn^{3+} / Mn^{4+} had direct impact on the strength of the ferromagnetic interactions.

12. Practical applicability, if any:

- The result obtained in both experimental and theoretical studies contribute to the knowledge about the origin of ferromagnetism in the Fe-doped manganites, the multi-ferroics with many important applications in the modern spintronics, so our results may be used directly in the process of the fabrication of the other novel compounds

13. Further research directions, if any:

- The study of the ferromagnetic transitions in low temperature region in the double perovskite system is very interesting object, which promises new important results about the phenomena still less understood such as the re-entrant spin glass state.

- The study of metallicity in the nanosize $CaMnO_3$ (under 5,4 nm) is an important direction. The appearance of ferromagnetism in the anti-ferromagnetic insulator materials is very interesting problem.

14. Thesis-related publications:

[1] Tran Thi Hong, Pham The Tan, Hoang Nam Nhat (2008), "Nanoparticles $CuMn_2O_4$ for methanol decomposition", *Enviromental science& technology for the earth,* Osaka, Japan*,* pp*.* 225-232.

[2] Vu Phuong Thanh, Nguyen Kien Cuong, Pham The Tan and Hoang Nam Nhat (2008), "Preparation, nanostructure, electronic and optical properties of the $CaCu_3Ti_4O_{12}$ ceramics with colossal dielectric constant", *Proceedings of APCTP–ASEAN Workshop on Advanced Materials Science and Nanotechnology*, p. 888-892.

[3] Pham The Tan, Tran Thi Hong, Hoang Nam Nhat (2009), "$Ca_3Mn_2O_7/TiO_2$ thin- film coating's effect on deactivation of biological pollutants", *Proceedings of* 6^{th} *SPMS , Da Nang, Vietnam, November 8-10,* pp. 1136-1139.

[4] Pham The Tan, Nguyen Kien Cuong, Fedor Valach and Hoang Nam Nhat (2009), "A simple method to estimate the spontaneous polarization in perovskite-like nanocrystallites"*, J Phys CS* 187*,* 012080*.*

[5] Hoang Nam Nhat, Pham The Tan (2010), "NMR in one-dimensional spin chains", *COMMAT-S* 49*,* S341-S347*.*

[6] Thuy Trang Nguyen, Thanh Cong Bach, Huong Thao Pham, The Tan Pham, Duc Tho Nguyen and Nam Nhat Hoang (2011), "Magnetic state of the bulk, surface and nanoclusters of $CaMnO_3$: A DFT study " *Physica B: Condensed Matter* 406 (19), pp. 3613-3621.

[7] Duc Huyen Yen Pham, The Tan Pham, Duc Tho Nguyen, Duc Thang Pham and Nam Nhat Hoang (2011), " Electronic structure of Fe-doped manganate $Ca(Fe_xMn_{1-x})O_3$ (x=0.01, 0.02, 0.03, 0.05)", *Proceedings of* 7^{th} *SPMS , Ho Chi Minh, Vietnam, November 7-9,* pp. 120-125.

[8] Tran Thi Hong, Pham The Tan , Hoang Nam Nhat *(2011)*, "On oxygen decifiency in nanocrystallites $La_{1-x}Sr_xCoO_3$", *e-J. Surf. Sci. Nanotech 9*. pp. 469-471.

[9] Duc Huyen Yen Pham, The Tan Pham, Duc Tho Nguyen, Duc Thang Pham and Nam Nhat Hoang (2013), "Optical Spectra of Colloidal Fe-doped Manganate $CaMn_{1-x}Fe_xO_3$ (x = 0, 0.01, 0.03, 0.05)", *Journal of the Korean Physical Society,* pp. 2133-2138.

[10] The-Tan Pham, Huyen-Yen Pham, Nam-Nhat Hoang and Nguyen Quang Hoa (2014), "Structure and Properties of Double Perovskite System $La_2Co_{1-x}Fe_xMnO_6$". *Communications in Physics*, Vol. 24, No. 3S1 (2014), DOI:10.15625/0868-3166/24/3S1/5224, pp. 80-84.