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ABSTRACTS

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GT-01. Structural stability and magnetic properties of the Mn-doped WS_2 thin films in *ab initio* calculations. *M. Kim*[1] and J. Hyun[1] *1. Sookmyung Womens University, Seoul, The Republic of Korea*

Two-dimensional (2D) transition-metal dichacogenides (TMDs) materials possess very interesting semiconducting, metallic, superconducting, and magnetic properties, which have been spurred lots of research in both experiment and theory to realize their advantageous features in, for example, the flexible and transparent electronics device applications. Among these TMDs, the nonmagnetic semiconductor WS_2 is one of the most exciting family of which the magnetic properties by transition metal doping exhibits exotic phenomena [1-4]. In this presentation, we report density functional theory (DFT) calculations on the Mn-doped WS_2 thin films, that is, monolayer and double layers. The spin magnetic moment of Mn-doped WS_2 monolayer is calculated to be 1.00 μ_B, respectively, at 4% impurity concentration in a 5×5 supercell. Upon the extension of the unit cell up to 7×7, we calculated the two Mn doped films to find the energy stability in accordance with the distance, which revealed that the nearest neighboring position on Mn atoms is most stable. Each total magnetic moment and Mn moments are 2.00 and 1.27 μ_B, respectively. We have examined the single as well as the double dopants of Mn in various probable interlayer doping positions using the structural stability and magnetic properties optimization and the formation energy calculations to decide the preferred doping sites as shown in Fig. 1. It was found that the single Mn dopant prefers the direct on-top positions (i) between the W atoms for the AA configuration (as shown in Fig 1(b)) and (ii) between the S and W atoms for the AB configuration (as in Fig 1(d)), to the hollow sites. The magnetic properties are also found to vary depending the configurations. *kimmy@sm.ac.kr **This work was supported by the Basic Science Research Program (No. 2017R1A2B4012972) through the National Research Foundation of Korea(NRF).

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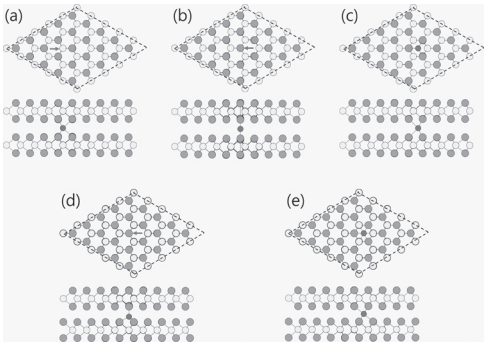

Fig. 1. Atomic models of a single Mn dopant in bilayer WS_2 with the (a) AA-W, (b) AA-S, (c) AA-H, (d) AB-WS, and (e) AB-H configurations. W, S, and Mn atoms are indicated by the yellow, gray, and red circles.

GT-02. Electronic and Magnetic Properties of Stoichiometric $CeAuBi_2$. M. Moda Piva[1,2], G. Silva Freitas[1], S.M. Thomas[2], J. Leao[3], *C. Adriano*[1], R.R. Urbano[1], J.W. Lynn[3], J. Thompson[2], P. Ferrari Silveira Rosa[2] and P. Pagliuso[1] *1. Instituto de Física "Gleb Wataghin" - UNICAMP, Campinas, Brazil; 2. Los Alamos National Laboratory, Los Alamos, NM, United States; 3. NIST Center for Neutron Research, Gaithersburg, MD, United States*

Rare-earth-based compounds have attracted attention of the scientific community as they are paradigms of multiple, often competing, interactions, such as the Ruderman-Kittel-Kasuya-Yoshida (RKKY) magnetic interactions, crystalline electrical field (CEF) effects, Kondo effect and Fermi surface effects. The interplay among these effects are complex and can lead to novel ground states. $CeAuBi_2$ is an example. It belongs to the $REMBi_2$ (RE = rare-earth, M = Cu, Au) family of antiferromagnets with competing magnetic interactions and, for RE = Ce, moderately heavy electrons [1-4]. Moreover, a breakdown of the de Gennes scaling for $CeMBi_2$ and $PrMBi_2$ implicates CEF enhancement of T_N [3, 4]. Furthermore, Au vacancies in some $CeAuBi_2$ materials indicate that disorder may also play an important role in this system [2]. Here we report the electronic and magnetic properties of stoichiometric $CeAuBi_2$ single crystals. $CeAuBi_2$ crystallizes in the tetragonal *P4/nmm* structure and orders antiferromagnetically below T_N = 19 K, the highest value reported for this compound [2, 4, 5]. At low temperatures (2 K) and ambient pressure, the application of magnetic fields parallel to the *c*-axis results in two transitions at 7.2 T and 7.7 T in the magnetoresistance, similar to $CeAuSb_2$ [6]. AC calorimetry and electrical resistivity experiments under pressure reveal that the application of external pressure favors antiferromagnetic order, which reaches a maximum T_N of 21 K at 23 kbar. Finally, neutron magnetic diffraction measurements find a commensurate antiferromagnetic structure with a propagation vector (0 0 1/2) with the magnetic moments aligned along the *c*-axis, similar to $CeCuBi_2$ [1].

[1] C. Adriano, P. F. S. Rosa, C. B. R. Jesus *et al.*, Phys. Rev. B, Vol. 90, p. 235120 (2014); [2] C. Adriano, P. F. S. Rosa, C. B. R. Jesus *et al.*, J. Appl. Phys., Vol. 117, p. 17C103 (2015); [3] C. B. R. Jesus, M. M. Piva, P. F. S. Rosa *et al.*, J. Appl. Phys., Vol. 115, p. 17E115 (2014); [4] C. B. R. Jesus, M. M. Piva, P. F. S. Rosa *et al.*, Phys. Procedia, Vol. 75, p. 618-624 (2015); [5] E. M. Seibel, W. Xie, Q. D. Gibson and R. J. Cava, J. Solid State Chem., Vol. 230, p. 318-324 (2015); [6] G. G. Marcus, D.-J. Kim, J. A. Tutmaher *et al.*, Phys. Rev. Lett., Vol. 120, p. 097201 (2018).

GT-03. The Effect of Manganese Substituted Sodium Iron Phosphate Maricite-$NaFe_{1-x}Mn_xPO_4$. *J. Seo*[1], H. Choi[1] and C. Kim[1] *1. Department of Physics, Kookmin University, Seoul, The Republic of Korea*

Transition metal ion substitution in sodium phosphate is effective in enhancing the performance of cathode material. [1] The Mn-doped maricite-$NaFe_{1-x}Mn_xPO_4$ (x = 0.1, 0.2, 0.3, 0.4, 0.5) samples were synthesized by solid-state route. The crystallographic and magnetic properties of the effect Mn substitution were investigated by x-ray diffraction (XRD) measurement, vibrating sample magnetometer (VSM), and Mössbauer spectroscopy. The XRD patterns of $NaFe_{1-x}Mn_xPO_4$ ($0.1 < x < 0.5$) revealed that the structure had orthorhombic structure with space group of *Pmnb*. The lattice parameters and the volume of the $NaFe_{1-x}Mn_xPO_4$ increased from for a_0 = 6.866, b_0 = 8.999, c_0 = 5.047 Å and V = 311.544 Å^3 for x = 0.1, a_0 = 6.881, b_0 = 9.037, c_0 = 5.075 Å and V = 315.418 Å^3 for x = 0.5. The temperature

dependence of the magnetization curves exhibits Néel temperature (T_N) of $NaFe_{1-x}Mn_xPO_4$ decreased with the increasing Mn concentrations from 14 K for x = 0.1 and 10 K for x = 0.5, indicating in weakened antiferromagnetic interaction. The Mössbauer spectra exhibited to have asymmetrical line-shapes below T_N and were fitted with eight Lorentzian lines, due to the strong crystalline field in the distorted $Fe(Mn)O_6$ octahedral site. At room temperature, exhibits a doublet absorption line. The decrease in antiferromagnetic order can be explained by the fact that the Fe-O-Mn interaction is weaker than the interaction of the paramagnetic region.

[1] T. Boyadzhieva, V. Koleva and R. Stoyanova, Phys.Chem.Chem.Phys., Vol. 19, p.12730 (2017)

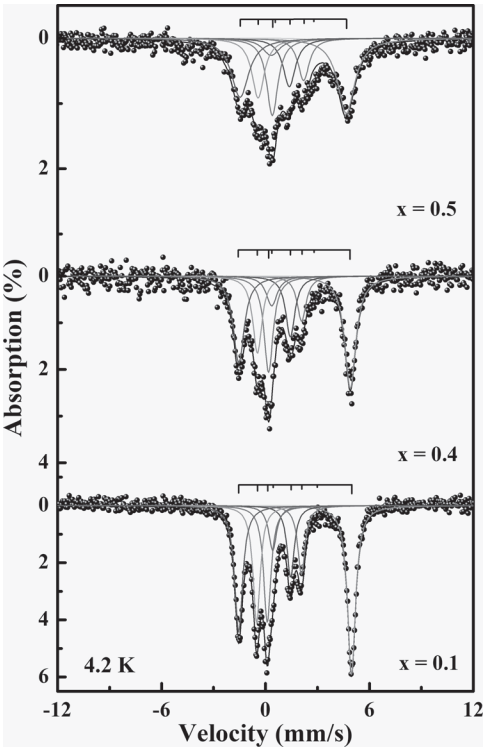

Fig 1. Mössbauer spectra of $NaFe_{1-x}Mn_xPO_4$ (x = 0.1, 0.4, 0.5) at 4.2 K.

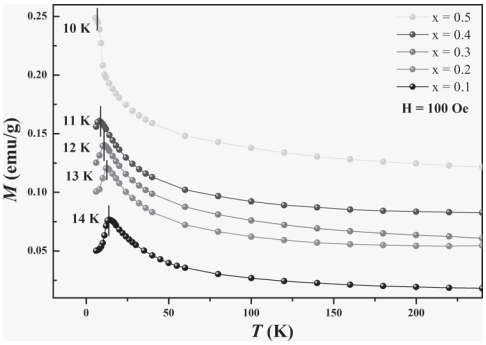

Fig 2. Temperature-dependent magnetization curve of the $NaFe_{1-x}Mn_xPO_4$ at various temperatures.

GT-04. Atomic-layer stacking dependence of the magnetocrystalline anisotropy and Dzyaloshinskii-Moriya interaction in Fe-Co multilayers on MgO. *Y. Kato*[1], A.M. Pradipto[1], T. Akiyama[1], T. Ito[1], T. Oguchi[2], M. Weinert[3] and K. Nakamura[1] *1. Engineering, Mie University, Tsu, Japan; 2. Scientific and Industrial Research, Osaka University, Suita, Japan; 3. Physics, University of Wisconsin-Milwaukee, Milwaukee, WI, United States*

For the next generation of magnetic tunnel junctions, control of the magnetocrystalline anisotropy (MCA) and the Dzyaloshinskii-Moriya interaction (DMI) in thin ferromagnetic films has attracted much attention. A promising approach to deal with such magnetic properties is by tuning the atomic-layer stacking sequences in multilayer thin films [1]. Here, we theoretically investigated the atomic-layer stacking dependence of the MCA and DMI in prototypical Fe-Co multilayer thin films on MgO(001). The generalized gradient approximation calculations were carried out using the film full-potential linearized augmented plane-wave method [2] employing single slabs with six-atomic layers of Co-Fe on MgO(001). The MCA energy is determined as difference in total energy for magnetizations oriented along the in-plane and perpendicular directions with respect to the film plane, and the DMI parameter of the multilayers is estimated from the total energy difference with respect to the spin-spiral wavevectors. The results predict that both MCA and DMI depend significantly on the atomic-layer stacking sequences. MCA energies, ranging from 1.4 [meV/unit-area] (perpendicular magnetization) to -1.5 [eV/unit-area] (in-plane magnetization), depending on the atomic-layer stacking sequences are observed. Similarly, complicated behavior of the DMI parameters versus the atomic-layer stacking sequences is observed, where the magnitude of the DMI parameter interestingly increases by one order of magnitude compared to that of pure Fe films even though the spin-orbit coupling is quite weak. We further analyze these magnetic properties by using cluster expansion and neural network methods in order to elucidated the underlying trends. We find that the MCA is very sensitive to the short-range order in the atomic-layer stacking sequences, whereas an asymmetry in the whole film along the stacking direction may play a role in determining the DMI.

[1] Hotta *et.al.,* Phys. Rev. Lett. 110, 267206 (2013) [2] Wimmer *et.al.*, Phys. Rev. B 24, 864 (1981), Weinert *et.al.*, Phys. Rev. B 26, 4571 (1982); Nakamura *et al.*, Phys. Rev. B 67, 014420 (2003).

GT-05. Effects of Simultaneous Cd and Ir Doping in Ce_2RhIn_8 Antiferromagnet. *D.S. Christovam*[1], G. Silva Freitas[1], M.M. Piva[1], J.C. Souza[1], J. Leao[2], W.D. Ratcliff[2], J.W. Lynn[2], P. Pagliuso[1] and C. Adriano[1] *1. DEQ, Instituto de Física Gleb Wataghin - Unicamp, Campinas, Brazil; 2. NIST Center for Neutron Research, NIST, Gaithersburg, MD, United States*

Ce_2RhIn_8 is an antiferromagnet (T_N = 2.8 K) that belongs to the family of Ce-based heavy fermion (HF) compounds Ce_mMIn_{3m+2} (*M* = Co, Rh, Ir). This family has been heavily investigated due to its intricate phase diagrams, which display complex magnetism, disordered phases and superconducting states [1,2]. These phase diagrams result from the competition between long-range Ruderman–Kittel–Kasuya–Yosida interaction, local on-site Kondo effect and crystalline electric field (CEF) effects, which have an important role in determining the ground state (GS) and physical properties of the compound [3]. The determination of the magnetic structure of these compounds is very helpful when studying the spin anisotropy of the CEF GS, since the moment direction can relate to its symmetry properties and magnetic anisotropy. The evolution of the physical properties of the $Ce_2Rh_{1-x}Ir_xIn_8$ series and the role of Cd doping in the Ce_2MIn_8 (*M* = Rh, Ir) site have been previously investigated [2,4]. It has been shown that Ir substitution seems to suppress the antiferromagnetism (AFM) and induce a coexisting superconducting phase, as well as a disordered spin-glass phase in the Ir-rich compounds. This evolution is accompanied by an enhancement of the Kondo effect and likely changes in the CEF scheme. On the contrary, Cd doping in Ce_2MIn_8 increases T_N favoring AFM for *M* = Rh and suppresses the superconductivity for *M* = Ir, suggesting that the main role of Cd in these systems is the electronic tuning of the GS, such as for the $CeMIn_5$