1. Biographical Data

S E X : male

Name in Full : CHANG HOON, LEE

Place of Birth : Kwang ju, Chonnam, KOREA

Citizenship: Korean

Present address : 434 Brook Arbor Dr, Cary, NC, 27519, USA

Phone: +1-919-465-1885

Office Address: Department of Chemistry, Cox Hall, Campus Box 8204, Raleigh, NC 27695-8204, USA

Phone: +1-919-515-2998

Fax: +1-919-515-2545

2. Educational Background

Degrees	Institution	Date
B.S	Department of Chemistry College of Natural and Sciences Wonkwang University	March 1991 - February 1998
M.S.	Department of Chemistry The Graduate School Wonkwang University	March 1998 - February 2000
Ph.D	Department of Chemistry The Graduate School Wonkwang University	March 2001 – July 2005
Post Doc	Department of Chemistry North Carolina State University	September 2005 – Aug. 2010
Research associate Professor	Department of Chemistry North Carolina State University	Dec. 2010 – Aug. 2011
Research associate Professor	Department of Chemistry POSTECH	Oct. 2011-present

3. Military Service

Branch of Service: Army, Period of Service: April, 1992 - July, 1994

4. Research background.

1) Electronic Band Structures of Low-Dimensional Metallic Compounds

In understanding the transport and other physical properties of low-dimensional metallic compounds, it is essential to know how their electronic structures are related to their crystal structures. In this project we attempt to provide theoretical understanding for transport, optical and structural properties of various low-dimensional conducting materials, which include transition-metal compounds and organic conducting salts. To achieve this objective, we carry out electronic band structure, density of state and Fermi surface calculations. To probe the structure-property relationships governing these compounds, the calculated electronic structures of these compounds are analyzed from the viewpoint of chemical concepts such as orbital interaction, overlap and symmetry.

2) Theoretical Study of Spin Exchange Interactions in Magnetic Solids

Physical properties of a magnetic solid are described by a spin-Hamiltonian, which is written in terms of pair-wise spin exchange interactions and the associated spin exchange parameters. When the magnetic susceptibility, neutron inelastic scattering or Raman scattering data of a magnetic solid are analyzed in terms of a spin-Hamiltonian, the spin exchange parameters are obtained as numerical fitting parameters needed to reproduce the experimental data. This project attempts to correlate such “experimental” parameters with the geometrical structure of a magnetic solid by performing electronic structure calculations for its spin dimers (i.e., the structural units containing two adjacent spin sites). In this project, the spin exchange parameters of a magnetic solid are determined using first principles electronic structure calculations. In addition, the trends in the spin exchange parameters of magnetic solids are explained on the basis of semi-empirical electronic structure calculations.

3) A multiferroic is a material in which two or all three of ferroelectricity, ferromagnetism and ferroelasticity occur in the same phase. The ferro describes a broken symmetry, and a related character, that can be aligned by application of an appropriate field: spontaneous magnetization, reoriented by an applied magnetic field; electric polarization, reoriented by an electric field; and spontaneous deformation, which can be reoriented by an applied stress. The coupling between ferroelectricity and ferroelasticity is well established, and leads to the widespread use of ferroelectric materials in transducer applications. Similarly the coupling between ferromagnetism and ferroelectricity results in magnetoelectricity and the manipulation of magnetic behavior by electric fields and vice versa. For a crystalline solid to exhibit ferroelectric polarization, it should not possess inversion symmetry. A centrosymmetric magnetic solid can lose inversion symmetry either by cooperative second-order Jahn-Teller distortion or by chiral magnetic order. In principle, a noncentrosymmetric magnetic solid can have ferroelectric polarization independent of its magnetic structure. For the noncentrosymmetric state brought about by a chiral magnetic order to readjust its charge distribution, SOC interactions are essential.

5. Awards

American Institutes of Chemists (AIC), USA 2008

6. Research interests

1) Chemical bonding in solid state materials

2) Theoretical Study of Spin Exchange Interactions in Magnetic Solids and Organometallic compounds.

3) Magnetic, Ferroelectric and Multiferroic materials.

4) Thermoelectric materials.

7. Research Experience.

Postdoctoral Associate Sep. 2005 ~ present

In the group of Professor Myung-Hwan Whangbo, Department of Chemistry, North Carolina State University.

1) Research on modified electron counting scheme for intermetallic compounds containing both electropositive elements (for example, alkaline-earth and rare-earth metals) and late transition metals. We discussed the results of our electronic-band structure calculations for three isostructural intermetallic compounds, La_2Ge_2In, La_2Pt_2In, and La_2Cu_2In. Our work has shown that the transition-metal atoms in La_2Pt_2In and La_2Cu_2In exist as the Zintl ions $[Pt\text{-}Pt]^{6-}$ and $[Cu\text{-}Cu]^{4-}$, respectively, and has clarified why the orbital sequence of a transition metal switches from nd < (n+1)s < (n+1)p to (n+1)s < nd < (n+1)p depending on its oxidation state. The transition-metal atoms in such compounds can be regarded as anions with bonding characteristics similar to those of the late main-group elements of Periods 4–6.

2) Research on multiferroic and spin frustrated systems. The spin frustration causing this magnetic structure of $Ba_3NbFe_3Si_2O_{14}$ was examined by evaluating its spin exchange interactions on the basis of density functional calculations and also by calculating its magnetic dipole-dipole interactions. The contribution of the chiral magnetic structure to the ferroelectric polarization of $Ba_3NbFe_3Si_2O_{14}$ below TN was estimated by Berry phase calculations. The spin exchanges of $Ba_3NbFe_3Si_2O_{14}$ are frustrated in each //ab sheet and between adjacent sheets of Fe^{3+} ions. The helical spin rotation along the c axis occurs to minimize the intersheet spin frustration as well as the intersheet magnetic dipole-dipole interactions. The ferroelectric polarization of $Ba_3NbFe_3Si_2O_{14}$ estimated from calculations is in good agreement with the experimental value.

3) Research on magnetic properties by using DFT and DFT+SOC (Spin-Orbit-Coupling). (a) For Cs_2CuCl_4 study, we reveals that despite a three-dimensional arrangement of its $CuCl_4^{2-}$ ions, the magnetic properties of Cs_2CuCl_4 are explained by a two-dimensional frustrated triangular antiferromagnetic spin lattice by evaluating the spin exchange interactions of A_2CuCl_4 (A = Cs, Rb, K, Na) on the basis of first principles density functional calculations. The observed magnetism of Cs_2CuCl_4 arises from this symmetry-dependent

participation of the 6p prbitals of the Cs^{+} ions in the spin exchange interactions between $CuCl_4^{2-}$ ions. (b) For $TbFe_3(BO_3)_4$ study, our studies indicates that the spin exchange between the Fe^{3+} spins is ferromagnetic within each //ab sheet of Fe^{3+} ions, but antiferromagnetic between adjacent //ab sheets of Fe^{3+} ions, while the spin exchange between the Fe^{3+} and Tb^{3+} ions within each //ab sheet of Fe^{3+} and Tb^{3+} ions is antiferromagnetic. The Tb^{3+} (f^8) ions is found to possess an electron configuration responsible for uniaxial magnetism, hence orienting the Tb^{3+} spins along the c-direction and leading to the highly anisotropic magnetic susceptibility. The ferroelectric polarization of $TbFe_3(BO_3)_4$ is due largely to the absence of inversion symmetry of the crystal structure, and is weakly affected by its magnetic structure.

4) Research on carbon cluster isomers. The geometrical structures and energetics of positively doubly charged fullerene dimer $(C_{60})_2{}^{2+}$ conformers were studied using semiempirical PM3 and MNDO, Hartree-Fock (HF), and Hybrid B3LYP density functional methods. The shape of the HOMO-LUMO for the three conformers was also analyzed. The *gauche* conformer was the most stable of the three conformers. The *anti* conformer was more stable than the *syn* conformer.

8. Computer skills

1) Computational Packages: VASP, WIEN2K, CEASAR, LMTO, GUASSIAN03
2) Programming Skills: Fortran90, C, python programming
3) Operating Systems: Linux, Unix, and Windows

9. Publications.

(1) M.-H. Whangbo, **C. Lee** and J. Köhler, "**Transition-metal anions in solids and their implications on bonding**", *Angew. Chem. Int. Ed*. **45**, 7465 (2006).

(2) J. Köhler, S. Deng, **C. Lee** and M.-H. Whangbo, "On the Origin of a Band Gap in Compounds of Diamond-like Structures", *Inorg. Chem.* **46**, 1957 (2007).

(3) H.-J. Koo, **C. Lee**, G. B. Wilson-Short, D. Dai and M.-H. Whangbo, "**On the Relevance of an Antiferromagnetic Dimer Model for the Spin-Gapped Magnetic Solids Cu(terpy)Mo_2O_7 and Cu(OH)(*p*-pyc)H_2O**", *Inorg. Chem.* **46**, 2498 (2007).

(4) **C. Lee**, M.-H. Whangbo and A. Villesuzanne, "On the electronic structure required for the uniaxial magnetic properties of the magnetic metal $SrCo_6O_{11}$", *Chem. Mater.* **19**, 2712 (2007).

(5) J. Köhler, H. A. Friedrich, **C. Lee**, and M.-H. Whangbo, "$IrIn_7GeO_8$ = $[IrIn_6](GeO_4)(InO_4)$ and compounds of the solid solution series $[IrIn_6](Ge_{1+x}In_{1-4x/3}O_8)$ ($0 \leq x \leq 0.75$): first oxides containing $[IrIn_6]$ octahedra", *Z. Anorg. Alleg. Chem*. **633**, 1464 (2007).

(6) **C. Lee**, M.-H. Whangbo and J. Köhler, "Stuffed graphite-like vs. stuffed diamond-like structures of the 18 valence electron compounds *RE*AuSn (*RE* = rare earth)", *Z. Anorg. Alleg. Chem*. **633**, 1464 (2007).

(7) K. H. Lee, R. Dieckmann, **C. Lee** and M.-H. Whangbo, "Predicting anisotropic electrical conductivities of a magnetic insulator on the basis of its magnetic properties", *Chem.Mater.* **19**, 4393 (2007).

(8) H. Ben Yahia, E. Gaudin, **C. Lee**, M.-H. Whangbo and J. Darriet, "Structural and magnetic properties of a new type of ordered oxygen-deficient perovskite, $KMnVO_4$", *Chem. Mater*. **19**, 5563 (2007).

(9) H. J. Xiang, **C. Lee** and M.-H. Whangbo, "On the absence of a spiral magnetic order in Li_2CuO_2 with one-dimensional CuO_2 ribbon chains", *Phys. Rev. B: Rapid Commun*. **76**, 220411(R) (2007).

(10) G. H. Chan, **C. Lee**, D. Dai, M.-H. Whangbo and J. A. Ibers, "On the Anisotropy of the Magnetic Properties of $CsYbZnSe_3$", *Inorg. Chem*. **47**, 1687 (2008).

(11) H. Kabbour, E. Janod, B. Corraze, M. Danot, L. Cario, **C. Lee** and M.-H. Whangbo, "Design, structure and physical properties of oxychalcogenides $A_2F_2Fe_2OX_2$ (A = Ba, Sr; X = Se, S) with Fe_2O square planar layer of the anti CuO_2-type", *J. Am. Chem. Soc*. **130**, 8261 (2008).

(12) X. Liu and R. Dronskowski, R. K. Kremer and M. Ahrens, **C. Lee** and .-H. Whangbo, "Characterization of the magnetic and structural properties of copper carbodiimide, CuNCN, by neutron diffraction and first-principles evaluations of its spin exchange interactions", *J. Phys. Chem. C*, , **112**, 11013 (2008).

(13) **C. Lee**, M.-H. Whangbo and J. Köhler, "Analysis of electronic structures and chemical bonding of metal-rich compounds. 1. Density functional study of Pt metal, $LiPt_2$, LiPt and Li_2Pt", *J. Comput. Chem*. **29**, 2154 (2008).

(14) M. Angst, R. P. Hermann, A. D. Christianson, M. D. Lumsden, **C. Lee**, M.-H. Whangbo, J.-W. Kim, P. J. Ryan, S. E. Nagler, W. Tian, R. Jin, B. C. Sales and D. Mandrus, "Charge order in LuFe2O4: antiferroelectric ground state and coupling to magnetism", *Phys. Rev. Lett*. **101**, 227601 (2008).

(15) J. L. Manson, M. M. Conner, A. C. McConnell, H. I. Southerland, J. A. Schlueter, I. Malfant, T. Lancaster, S. J. Blundell, M. L. Brooks, F. L. Pratt, J. Singleton, R. D. McDonald, **C. Lee** and M.-H. Whangbo, "Experimental and theoretical characterization of the magnetic properties of $CuF_2(H_2O)_2$(pyz) (pyz = pyrazine): A two-dimensional quantum magnet arising from super-superexchange interactions through hydrogen bonded paths", *Chem. Mater*. **20**, 7409 (2008).

(16) R. Dessapt, M. Collet, V. Coué, M. Bujoli-Doeuff, S. Jobic, **C. Lee** and M.-H. Whangbo, "Kinetics of Coloration in Photochromic Organoammonium Polyoxomolybdates", *Inorg. Chem*. **48**, 574 (2009).

(17) J. L. Manson, K. H. Stone, H. I. Southerland, T. Lancaster, A. J. Steele, S. J. Blundell, F. L. Pratt, P. J. Baker, R. D. McDonald, P. Sengupta, J. Singleton, P. A. Goddard, **C. Lee**, M.-H. Whangbo, M. M. Warter, C. H. Mielke and P. W. Stephens, "Characterization of the antiferromagnetism in $Ag(pyz)_2(S_2O_8)$ (pyz = pyrazine) with a two-dimensional square lattice of Ag^{2+} ions", *J. Am. Chem. Soc*. **131**, 4590 (2009).

(18) **C. Lee**, J. Kang, K. H. Lee and M.-H. Whangbo, "Symmetry-dependent strong reduction of the spin exchange interactions in Cs_2CuCl_4 by the 6p orbitals of Cs^+ ions", *Inorg. Chem*. **48**, 4185 (2009).

(19) J. L. Manson, J. A. Schlueter, K. A. Funk, H. I. Southerland, B. Twamley, T. Lancaster, S. J. Blundell, P. J. Baker, F. L. Pratte, J. Singleton, R. D. McDonald, P. A. Goddard, P. Sengupta, C. D. Batista, L. Ding, **C. Lee**, M.-H. Whangbo, I. Franke, S. Cox, C. Baines, and D. Triala, "Strong H···F hydrogen bonds as synthons in polymeric quantum magnets: Structural, magnetic and theoretical characterization of $[Cu(HF_2)(pyrazine)_2]SbF_6$, $[Cu_2F(HF)(HF_2)(pyrazine)_4](SbF_6)_2$ and $[CuAg(H_3F_4)$ $(pyrazine)_5](SbF_6)_2$", *J. Am. Chem. Soc*. **131**, 6733 (2009).

(20) **C. Lee**, J. Kang, K. H. Lee and M.-H. Whangbo, "Density functional investigation of the antiferromagnetic ordering, spin orientation and ferroelectric polarization of rare-earth iron borate $TbFe_3(BO_3)_4$", *Chem. Mater*. **21**, 2534 (2009).

(21) M. G. Banks, R. K. Kremer, C. Hoch, A. Simon, B. Ouladdiaf, J.-M. Broto, H. Rakoto, **C. Lee**, and M.-H. Whangbo, "Magnetic ordering in the frustrated Heisenberg chain system cupric chloride $CuCl_2$", *Phys. Rev. B* **80**, 024404 (2009).

(22) J. Kang, **C. Lee**, R. K. Kremer and M.-H. Whangbo, "Consequences of the intrachain dimer-monomer spin frustration and the interchain dimer-monomer spin exchange in the diamond-chain compound Azurite $Cu_3(CO_3)_2(OH)_2$", *J. Phys.:Condens. Matter*, **21**, 392201 (2009).

(23) E. J. Kan, H. J. Xiang, Y. Zhang, **C. Lee** and M.-H. Whangbo, "Density functional analysis of the spin exchange and the ferroelectric polarization in $AgCrO_2$", *Phys. Rev. B*, **80**, 104417 (2009).

(24) H.-J. Koo, H. J. Xiang, **C. Lee**, and M.-H. Whangbo, "Effect of Magnetic Dipole-Dipole Interactions on the Spin Orientation and Magnetic Ordering of the Spin Ladder Compound $Sr_3Fe_2O_5$", *Inorg. Chem*. **48**, 9051 (2009).

(25) C. Tian, **C. Lee**, H. J. Xiang, Y. Zhang, C. Payen, S. Jobic, and M.-H.Whangbo, "Magnetic structure and ferroelectric polarization of $MnWO_4$ investigated by density functional calculations and classical spin analysis", *Phys. Rev. B*, **80**, 104426 (2009).

(26) J. L. Musfeldt, L. I. Vergara, T. V. Brinzari, **C. Lee**, L. C. Tung, J. Kang, Y. J. Wang, J. A. Schlueter, J. L. Manson and M.-H. Whangbo, "Magnetoelastic interactions in a two-dimensional quantum antiferromagnet", *Phys. Rev. Lett*., **103**, 157301 (2009).

(27) O. Mentré, E. Janod, P. Rabu, M. Hennion, F.Leclercq-Hugeux, J. Kang, C. Lee, M.-H. Whangbo and S. Petit, "$BiCu_2PO_6$: Frustration driven incommensurate dispersion in a gapp ed quantum spin ladder", *Phys. Rev. B* **80**, 180413 (2009).

(28) J. L. Manson, T. Lancaster, S. J. Blundell, Y. M. Qiu, J. Singleton, P. Sengupta, F. L. Pratt, J. Kang, **C. Lee** and M.-H. Whangbo, "Spin fluctuations and orbital ordering in quasi-one-dimensional alpha-$Cu(dca)_2(pyz)$ {dca = dicyanamide = $N(CN)_2^-$; pyz = pyrazine}, a molecular analogue of $KCuF_3$", *Polyhedron*, **29**, 514 (2010).

(29) **C. Lee**, M.-H. Whangbo and J. Köhler, "Analysis of electronic structures and chemical bonding of metal-rich compounds. 2. Presence of dimer $(T\text{-}T)^{4-}$ and isolated T^{2-} anions in the polar intermetallic Cr_5B_3-type compounds AE_5T_3 (*AE* = Ca, Sr; T = Au, Ag, Hg, Cd, Zn)", *Z. Anorg. Allge. Chem*. **636**, 36 (2010).

(30) E. J. Kan, H. J. Xiang, **C. Lee**, F. Wu, J. L. Yang and M.-H. Whangbo, "Origin of the ferroelectricity in pervoskites with s^0 A-site cations: Toward Near-Room-Temperature Multiferroics", *Angew. Chem. Int. Ed.* **49**, 1603 (2010).

(31) K. Tomiyasu, H. Kageyama, **C. Lee**, M.-H. Whangbo, Y. Tsujimoto, T. Watanabe, K. Yoshimura, J. W. Taylor, A. Llobet, F. Trouw, K. Kakurai and K. Yamada, "Magnetic Excitations in Infinite-Layer Antiferromagnetic Insulator ", *J. Phys. Soc. Jpn*., **79**(3), 034707 (2010).

(32) J. L. White, **C. Lee**, Ö . Günaydin-Şen, L. C. Tung, H. M. Christen, Y. J. Wang, M. M. Turnbull, C. P. Landee, R. D. McDonald, S. A. Crooker, J. Singleton, M.-H. Whangbo and J. L. Musfeldt, "Magneto-optical properties and charge-spin coupling in the molecular $(2,3\text{-dmpyH})_2CuBr$ spin-ladder material", *Phys. Rev. B.*, **81**(5), 152407 (2010)

(33) J. Tong, **C. Lee**, M.-H. Whangbo, R. K. Kremer, A. Simon and J. Köhler, "Cooperative Jahn-Teller distortion leading to the spin-1/2 uniform antiferromagnetic chains in triclinic perovskites $AgCuF_3$ and $NaCuF_3$", *Solid State Sci*., **12**(5), 680 (2010).

(34) Ö. Gunaydın-Şen, **C. Lee**, L. C. Tung, P. Chen, M. M. Turnbull, C. P. Landee, Y. J. Wang, M.-H. Whangbo, and J. L. Musfeldt, "Spin-lattice interactions through the quantum critical transition in $Cu(pyz)(NO_3)_2$" *Phys. Rev. B.*, **81**(10), 104307 (2010).

(35) Chuan Tian, Erjun Kan, Changhoon Lee, and Myung-Hwan Whangbo, "π-Back-Donation Effect of the Cyanide Ligands on the Electron Correlation and Charge Transfer in Prussian Blue $RbMn[Fe(CN)_6]$", *Inorg. Chem*. **49**(7), 3086 (2009).

(36) Changhoon Lee, Sung Soo Park, Wang Ro Lee, and Kee Hag Lee, "Structure and Energetics of $(C_{60})_2^{2+}$ Conformers: Quantum Chemical Studies", *The Bulletin of the Korean Chemical Society*, 31(2), 457 (2010).

(37) E. J. Kan, H. J. Xiang, F. Wu, C. Tian, **C. Lee**, J. L. Yang, and M.-H. Whangbo, "Prediction for room-temperature half-metallic ferromagnetism in the half-fluorinated single layers of BN and ZnO" *APPLIED PHYSICS LETTERS***,** **97**, 122503 (2010).

(38) Erjun Kan, Hongjun Xiang, Fang Wu, **Changhoon Lee**, Jinlong Yang, and Myung-Hwan Whangbo, "Ferrimagnetism in zigzag graphene nanoribbons induced by main-group adatoms" *APPLIED PHYSICS LETTERS*, **96**, 102503 (2010).

(39) Changhoon Lee, Erjun Kan, Hongjun Xiang, and Myung-Hwan Whangbo, "Theoretical Investigation of the Magnetic Structure and Ferroelectric Polarization of the Multiferroic Langasite $Ba_3NbFe_3Si_2O_{14}$" *Chem. Mater*. **22**(18) , 5290 (2010).

(40) Tassel, C.; Kang, J.; Lee, C.; Hernandez, O.; Qiu, Y.; Paulus, W.; Collet, E.; Lake, B.; Guidi, T.; Whangbo, M.-H.; Ritter, C.; Kageyama, H.; Lee, S.-H.
"Ferromagnetically coupled Shastry-Sutherland quantum spin singlets in (CuCl)$LaNb_2O_7$." *Physical Review Letters*, **105**(16), 167205/1-167205/4 (2010)

(41) Manson, Jamie L.; Warter, Michelle L.; Schlueter, John A.; Lancaster, Tom; Steele, Andrew J.; Blundell, Stephen J.; Pratt, Francis L.; Singleton, John; McDonald, Ross D.; Lee, Changhoon; Whangbo, Myung-Hwan; Plonczak, Alex.
"[$Cu(HF_2)_2$(pyrazine)]$_n$: A Rectangular Antiferromagnetic Lattice with a Spin Exchange Path Made Up of Two Different FHF- Bridges." *Angewandte Chemie, International Edition* , **50**(7), 1573-1576 (2011)

(42) Tong, Jianwei; Kremer, Reinhard K.; Koehler, Juergen; Simon, Arndt; Lee, Changhoon; Kan, Erjun; Whangbo, Myung-Hwan.
"The layered ferromagnet Cs_2AgF_4: antiferromagnetic inter-layer coupling driven by magnetic dipole-dipole interactions." *Zeitschrift fuer Kristallographie (ZAAC)*, **225**(11), 498-503 (2011)

(43) Tian, Chuan; Lee, Changhoon; Kan, Erjun; Wu, Fang; Whangbo, Myung-Hwan. **"Analysis of the Magnetic Structure and Ferroelectric Polarization of Monoclinic MnSb2S4 by Density Functional Theory Calculations."** *Inorganic Chemistry*, **49**(23), 10956-10959 (2010)

(44) Kan, Erjun; Wu, Fang; Lee, Changhoon; Kang, Jinhee; Whangbo, Myung-Hwan. **"On the High Magnetic-Ordering Temperature of the 5d Magnetic Oxide Ca3LiOsO6 Crystallizing in**

a Trigonal Crystal Structure: Density Functional Analysis.” *Inorganic Chemistry*, **50**(9), 4182-4186 (2011)

(45) Koo, Hyun-Joo; Lee, Changhoon; Whangbo, Myung-Hwan; McIntyre, Garry J.; Kremer, Reinhard K. **“On the nature of the spin frustration in the CuO2 ribbon chains of LiCuVO4: crystal structure determination at 1.6 K, magnetic susceptibility analysis, and density functional evaluation of the spin exchange constants.**” *Inorganic Chemistry*, **50**(8), 3582-3588 (2011)

(46) H. J. Xiang, E. J. Kan, M.-H. Whangbo, C. Lee, Su-Huai Wei, and X. G. Gong. “**Single-ion anisotropy, Dzyaloshinskii-Moriya interaction, and negative magnetoresistance of the spin-1/2 pyrochlore *R*2V2O7**” *Phys. Rev. B*, **83**, 174402 (2011)

(47) Erjun Kan, Fang Wu, Changhoon Lee, Jinhee Kang, and Myung-Hwan Whangbo., “**On the High Magnetic-Ordering Temperature of the 5d Magnetic Oxide Ca3LiOsO6 Crystallizing in a Trigonal Crystal Structure: Density Functional Analysis”** *Inorg. Chem.*, *50* (9), 4182–4186 (2011)

(48) Lee, Jihyun; Lee, Changhoon; Park, Sung S.; Lee, Kee Hag. **“Full geometry optimizations of bond-stretch isomers of C202+ fullerene dication by the hybrid density functional B3LYP methods.”** Bulletin of the Korean Chemical Society 32(1), 277-280 (2011)

(49) C. Lee, E.J. Kan, M.-H. Whangbo, A. Bussmann-Holder A. Simon**, “Spin/Charge Redistributions and Oxygen Atom Displacements Induced by Spin Flip and Hole Doping in the CuO2 Layer of High-Temperature Superconductors”**
J Supercond Nov Magn “DOI 10.1007/s10948-011-1208-3”

(50) J. L. Musfeldt, Z. Liu, S. Li, J. Kang, C. Lee, P. Jena, J. L. Manson, J. A. Schlueter, G. L. Carr, and M.-H. Whangbo.**“Pressure-Induced Local Structure Distortions in Cu(pyz)$F_2(H_2O)_2$**” Inorg. Chem. 2011, 50, 6347–635.

(51) Myung-Hwan Whangbo, Changhoon Lee, Jürgen Köhler, “**Metal Anions in Metal-Rich Compounds and Polar Intermetallics**” *Eur. J. Inorg. Chem.* **2011**, 3841–3847.

(52) J. M. Law, P. Reuvekamp, R. Glaum, C. Lee, J. Kang, M.-H. Whangbo, and R. K. Kremer “**Quasi-one-dimensional antiferromagnetism and multiferroicity in CuCrO4”** PHYSICAL REVIEW B 84, 014426 (2011)

(53) J. M. Law, C. Hoch, R. Glaum, I. Heinmaa, R. Stern, J. Kang, C. Lee, M.-H. Whangbo, and R. K. Kremer, "**Spin-Peierls transition in the *S* = 1/2 compound TiPO4 featuring large intrachain coupling"** PHYSICAL REVIEW B 83, 180414(R) (2011)

(54) Jamie L. Manson, Saul H. Lapidus, Peter W. Stephens, Peter K. Peterson, Kimberly E. Carreiro, Heather I. Southerland, Tom Lancaster, Stephen J. Blundell, Andrew J. Steele, Paul A. Goddard, Francis L. Pratt, John Singleton,^ Yoshimitsu Kohama, Ross D. McDonald, Rico E. Del Sesto, Nickolaus A. Smith,O Jesper Bendix, Sergei A. Zvyagin, Jinhee Kang, Changhoon Lee, Myung-Hwan Whangbo, Vivien S. Zapf, and Alex Ploncza, "**Structural, Electronic, and Magnetic Properties of Quasi-1D Quantum Magnets [Ni(HF2)(pyz)2]X (pyz = pyrazine; X = PF6–, SbF6–) Exhibiting Ni-FHF-Ni and Ni-pyz-Ni Spin Interactions**" *Inorg. Chem*., **50**, 5990–6009 (2011)