Exploration of New Hybrid Solids that Display Magnetic Behavior Due to Confined Spins

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The research in Prof. Hwu's group deals with exploratory synthesis of solid state materials of catalytic, electronic and magnetic importance. The objective of the group research is threefold: 1) to explore new solid state compounds that possess novel structures and properties, 2) to evaluate and identify materials that have superior and/or enhanced physical and chemical properties for device applications, 3) to draw correlations between structure and property of newly synthesized solids for the fundamental study of the origin of unusual phenomena. One specific focus area is the exploration of new hybrid solids that contain low-dimensional magnetic nanostructures with high-spin values (*S*). Like molecular magnets, they exhibit unusual (size and geometry dependent) magnetic behaviors due to "confined" spins. Of particular interest are those systems containing transition metal and rare-earth metal cations exhibiting rich structure and/or redox chemistry. Compound characterizations will be directed toward revealing and understanding the bond strength, spin-spin and spin-lattice interactions, and band structures of quantized metal-oxide frameworks. The underlined research goal is to evaluate and determine the parameters that are critical for materials selection in quantum device applications, specifically for information storage and quantum computing. This research covers a broad range of fundamental inorganic chemistry in an emerging field of advanced materials.

PUBLICATIONS (with undergraduates in the last 5 years)

1. "Salt-Inclusion Synthesis of Two New Polar Solids $Ba_6Mn_4Si_{12}O_{34}Cl_3$ and $Ba_6Fe_5Si_{11}O_{34}Cl_3$," X. Mo, E. Ferguson,* S.-J. Hwu, *Inorg. Chem.*, **44**, 3121-3126. (2004).
2. "Synthesis, Structure and Magnetic Properties of $Cs_{2-x}Rb_xCu_3P_4O_{14}$ ($0.0 \leq x \leq 0.8$): A New Series of Copper(II) Phosphates Containing Periodic Arrays of Stagered Square Planar CuO_4 Trimers," K. G. S. Ranmohotti, X. Mo, M. K. Smith,* S.-J. Hwu, *Inorg. Chem.,* **45**, 3665-3670 (2006).

PRESENTATIONS (with undergraduates in the last 5 years)

1. "Hydrothermal Synthesis and Characterization of Manganese Oxide Open-Frameworks Using Salt-Lattice Templating," Matthew S. Williams,* Xunhua Mo, S.-J. Hwu, presented at the 17th National Conference on Undergraduate Research, Salt Lake City, Utah, March 13-15, 2003.
2. "Synthesis and Characterization of CU-6, a New Series of Layered Cuprates with Kagome Copper Network: $(CsX)\cdot Cu_5O_2(M'O_4)$ (X = Cl, Br, I; M' = P, As)," B. Alderman,* X. Mo, S.-J. Hwu, presented as a poster at the SURP Symposium, Clemson University, Clemson, SC, July 25, 2003.
3. "Salt Inclusion Synthesis of a Novel Series of Layered Transition Metal Silicates and Germanates," X. Mo, E. Ferguson,* S.-J. Hwu, presented at the 55th Southeast Regional Meeting of the American Chemical Society, Atlanta, GA, November 16-19, 2003.
4. "$(CsX)\cdot Cu_5O_2(AsO_4)_2$ (X = Cl, Br, I): A New Family of Salt-Inclusion Solids, CU-6. Novel Layered Cuprates with Kagome Network of a Pyrochlore-Type," M. Ulutagay-Kartin, X. Mo, Q. Huang, B. Alderman, E. Ferguson,* S.-J. Hwu, H.-J. Koo, M.-H. Whangbo and M. Krawiec, presented at the Gordon Research Conference on Solid State Chemistry, Colby-Sawyer College, July 25 - 30, 2004.
5. "$KCrAs_2O_7$ – A Missing Link in the $ACrX_2O_7$ Structure Family," A. Siegfried, A. Flowers,* L. Wang, S.-J. Hwu, presented at the 56th Southeast Regional Meeting of the American Chemical Society, Research Triangle Park, NC, November 10-13, 2004.
6. "$Cs_5K_4Fe_7(PO_4)_{10}$: A Novel Iron(III) Phosphate Exhibiting Intersecting Channels," G. Becht,* R. Britt, C. Eagle, S.-J. Hwu, presented at the 231st ACS National Meeting, Atlanta, GA, March 26-30, 2006.
7. "Li^+-Exchange and Redox Chemistry of Two New Iron(III)-Containing Mixed-Framework Solids $(K_{3-x}Cs_x)Fe_3(AsO_4)_4$ (x = 0.55) and $Cs_5K_4Fe_7(PO_4)_{10}$," Gregory A. Becht, Robin Britt,* Cassandra Eagle, Jack Vaughey, S.-J. Hwu, presented (poster) at the North American Solid State Chemistry Conference, Texas A&M University, College Station, TX, May 17-19, 2007.