

# Lebenslauf



## Dr. rer. nat. Manfred Speldrich

### Persönliche Daten

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Geburtsdatum	22. April 1966 in Jülich
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### Studium

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03/1989 – 04/2002	Hauptstudium im Diplomstudiengang Chemie an der RWTH Aachen University, Abschluss: Diplom in Chemie
04/2002 – 10/2002	Diplomarbeit am Institut für Anorganische Chemie der RWTH Aachen University, Titel: Magnetochemie von 5f <sup>N</sup> -Systemen
11/2002 – 05/2008	Dissertation (Dr. rer. nat.) am Institut für Anorganische Chemie der RWTH Aachen University in der Arbeitsgruppe von Prof. Dr. H. Lueken, Titel der Arbeit: Magnetochemische Analyse und Modellierung von d <sup>N</sup> -, 4f <sup>7</sup> - und 5f <sup>N</sup> -Systemen mit dem Computerprogramm CONDON
10/2003	Gastwissenschaftler am Paul Scherrer Institut (PSI), Schweiz, in der Arbeitsgruppe von Prof. Dr. A. Furrer
seit 05/2008	Wissenschaftlicher Mitarbeiter (Postdoc) am Inst. f. Anorg. Chemie der RWTH Aachen in der Arbeitsgruppe von Prof. Dr. P. Kögerler
09/2009	Gastwissenschaftler am Ames Laboratory, USA, in der Arbeitsgruppe von Prof. Dr. M. Luban
seit 09/2011	Praktikumsleiter für die lehramtsbezogenen Bachelorstudiengänge am Institut für Anorganische Chemie

## Publikationen 2004 – 2009

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- (1) H. Schilder, M. Speldrich, H. Lueken, A.C. Sutorik, M.G. Kanatzidis; The valence state of uranium in  $K_6Cu_{12}U_2S_{15}$ , *J. Alloys Comp.* **2004**, 374, 249-252.
- (2) I. Stein, M. Speldrich, H. Schilder, H. Lueken, U. Ruschewitz;  $^1_\infty[M(Py)_2(H_2O)_n(ADC)_{2/2}]$   $M \cong Fe, Co$  und  $Ni$  ( $n=2$ ) und  $M^{II} \cong Cu$  ( $n=1$ ) Vier neue Koordinationspolymere mit dem Acetylendicarboxylat-Dianion ( $ADC^{2-}$ ) als verbrückendem Liganden, *Z. Anorg. Allg. Chem.* **2007**, 633, 1382-1390.
- (3) M. Krott, X. Liu, B. Fokwa, M. Speldrich, H. Lueken, R. Dronskowski; Synthesis, Crystal-Structure Determination and Magnetic Properties of Two New Transition-Metal Carbodiimides:  $CoNCN$  and  $NiNCN$ , *Inorg. Chem.* **2007**, 46, 2204-2207.
- (4) M. A. J. Hodenius, T. Niendorf, G. A. Krombach, W. Richtering, T. Eckert, H. Lueken, M. Speldrich, R. W. Günther, M. Baumann, H. S. J. Soenen, M. De Cuyper, T. Schmitz-Rode; Synthesis, physicochemical characterization and MR relaxometry of aqueous ferrofluids *J. Nanosci. Nanotechnol.* **2008**, 8, 2399-2409.
- (5) F. Hussain, R. W. Gable, M. Speldrich, P. Kögerler, C. Boskovic; Polyoxotungstate-Encapsulated  $Gd_6$  and  $Yb_{10}$  Spin Clusters, *Chem. Commun.* **2009**, 3, 328-330.
- (6) X. Liu, L. Stork, M. Speldrich, H. Lueken, R. Dronskowski;  $FeNCN$  and  $Fe(NCNH)_2$ : Synthesis, Structure and Magnetic Properties of a Nitrogen-Based Pseudo-oxide and -hydroxide of Divalent Iron *Chemistry - A European Journal*, **2009**, 15, 1558-1561.
- (7) I. L. Malaestean, M. Speldrich, A. Ellern, S. G. Baca, H. Schilder, P. Kögerler; Synthesis, crystal structures and properties of new cobalt(II) linear trimer and 2D coordination polymer based on diphenic acid and diamines, *Eur. J. Inorg. Chem.* **2009**, 8, 1011-1118.
- (8) F. Hussain, B. Spingler, F. Conrad, M. Speldrich, P. Kögerler, C. Boskovic, G.R. Patzke; Cesium templated hexanuclear lanthanoid based polytungstoarsenate (III) clusters, *Dalton Transactions*, **2009**, 23, 4423-4425.
- (9) A. Wutkowski, Ch. Näther, M. Speldrich, P. Kögerler, W. Bensch; A Novel Expansion Mode of Polyoxovanadate Clusters: Synthesis, Crystal Structure and Properties of  $[Cu(H_2O)(C_5H_{14}N_2)_2]_2[V_{16}O_{38}(Cl)] \cdot 4(C_5H_{16}N_2)$  *Z. Anorg. Allg. Chem.* **2009**, 635, 1094-1099.
- (10) S. Biswas, M. Tonigold, M. Speldrich, P. Kögerler, D. Volkmer; Nonanuclear Coordination Compounds Featuring  $M_9L_{12}^{6+}$  Cores ( $M = Ni^{III}, Co^{II}$ , or  $Zn^{II}$ ;  $L = 1,2,3$ -Benzotriazolate) *Eur. J. Inorg. Chem.*, **2009**, 21, 3094-3101.
- (11) J. Beck, R. Glaum, P. Kögerler, M. Speldrich, Y. Ben-Amer; Transition Metal Terathiosquarates: One-Dimensional Linking in the  $Fe(II)$  salt  $FeC_4S_4 \times 6H_2O$  *Z. Anorg. Allg. Chem.* **2009**, 21, 1991-1996.
- (12) I. L. Malaestean, M. Speldrich, A. Ellern, S. G. Baca, M. Ward, and P. Kögerler; Decanuclear Manganese Isobutyrate Clusters Featuring a Novel  $Mn_8^{II}Mn_2^{III}$  Core, *Eur. J. Inorg. Chem.* **2009**, 28, 4209-4212.

## Publikationen 2010

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- (1) I. L. Malaestean, V. C. Kravtsov, M. Speldrich, G. Dulcevscaia, Y. A. Simonov, J. Lipkowski, A. Ellern, S. G. Baca, P. Kögerler; One-Dimensional Coordination Polymers from Hexanuclear Manganese Carboxylate Clusters Featuring a  $\{\text{Mn}_4^{\text{II}}\text{Mn}_2^{\text{III}}(\mu_4-\text{O})_2\}$  Core and Spacer Linkers *Inorg. Chem.* **2010**, 49, 7764–7772.
- (2) C. Ritchie, E. G. Moore, M. Speldrich, P. Kögerler, C. Boskovic; Terbium Polyoxometalate Organic Complexes: Correlation of Structure with Luminescence Properties, *Angew. Chem. Int. Ed.* **2010**, 49, 7702-7705.
- (3) I. L. Malaestean, M. Speldrich, A. Ellern, S. G. Baca, P. Kögerler; Heterometallic hexanuclear isobutyrate clusters based on di- and tripodal alcohols *Polyhedron* **2010**, 29, 1990–1997.
- (4) X. Liu, M. Speldrich, P. Kögerler, R. Dronskowski, A. L. Tchougreeff; Synthesis, Characterization, and Quantum-Chemical Studies of  $\text{Ni}(\text{CN})_2\text{MX}$  ( $\text{M} = \text{Rb}, \text{Cs}; \text{X} = \text{Cl}, \text{Br}$ ) *Inorg. Chem.* **2010**, 49, 7414-7423.
- (5) M. Albrecht, M. Fiege, P. Kögerler, M. Speldrich, R. Fröhlich, M. Engeser; Ferro- and antiferro-magnetic coupling in enantiomerically pure trinuclear helicate-type complexes formed by hierarchical self-assembly *Chem. Eur. J.* **2010**, 16, 8797-8804.
- (6) Y.-Z. Zheng, M. Speldrich, P. Kögerler, X.-M. Chen; The role of  $\pi - \pi$  stacking in stabilising the a,a-trans-cyclohexane-1,4-dicarboxylate in a 2D Co(II) network, *Cryst Eng Comm.*, **2010**, 12, 1057-1059.
- (7) L. Stork, P. Mueller, M. Speldrich, P. Kögerler, J. von Appen, R. Dronskowski; Synthesis, High-resolution Crystal Structure Refinement and Magnetic Properties of the Manganese-rich Cementite-type  $\text{Mn}_{1.8}\text{Fe}_{1.2}\text{C}$  *Z. Naturforsch. B* **2010**, 65, 1235-1239.
- (8) D. Wandner, P. Link, O. Heyer, J. Mydosh, M. A. Ahmida, M. M. Abd-Elmeguid, M. Speldrich, H. Lueken, U. Ruschewitz; Structural Phase Transitions in  $\text{EuC}_2$ , *Inorg. Chem.* **2010**, 49, 312.
- (9) X. Fang, M. Speldrich, H. Schilder, R. Cao, K. P. O'Halloran, C. L. Hill, P. Kögerler; Switching slow relaxation in a  $\text{Mn}_3^{\text{III}}\text{Mn}^{\text{IV}}$  cluster: an example of grafting single-molecule magnets onto polyoxometalates *Chem. Commun.* **2010**, 46, 2760-2762.
- (10) S. Biswas, M. Tonigold, M. Speldrich, P. Kögerler, M. Weil, D. Volkmer; Syntheses and Magnetostructural Investigations on Kuratowski-Type Homo- and Heteropen-tanuclear Coordination Compounds  $[\text{MZn}_4\text{Cl}_4(\text{L})_6]$  ( $\text{M}^{\text{II}} = \text{Zn}, \text{Fe}, \text{Co}, \text{Ni}, \text{or Cu}$ ;  $\text{L} = 5,6\text{-Dimethyl-1,2,3-benzotriazolate}$ ) Represented by the Nonplanar  $K_{3,3}$  Graph *Inorg. Chem.* **2010**, 49, 7424-7434.
- (11) X. Tang, H. Xiang, X. Liu, M. Speldrich, R. Dronskowski; The first ferromagnetic carbodiimide:  $\text{Cr}_2(\text{NCN})_3$  *Angew. Chem. Int. Ed.*, **2010**, 49, 4738–4742.
- (12) Y.-Z. Zheng, M. Speldrich, H. Schilder, X.-M. Chen, P. Kögerler; A tetranuclear cobalt(II) chain with slow magnetization relaxation, *Dalton Transactions* **2010**, 39, 10827-10829.

## Publikationen 2011

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- (1) S. G. Baca, O. Botezat, I. Filippova, M. Speldrich, E. Jeanneau, P. Kögerler; A Heptanuclear Iron(III) Oxo-Carboxylate Cluster *Z. Anorg. Allg. Chem.* **2011**, 637, 821-823
- (2) F. Xikui, P. Kögerler, Y. Furukawa, M. Speldrich, M. Luban; Molecular Growth of a Core-Shell Polyoxometalate *Angew. Chem. Int. Ed.* **2011**, 50, 5212-5216.
- (3) S. G. Baca, M. Speldrich, A. Ellern, P. Kögerler;  $\{Fe_6O_2\}$ -Based Assembly of a Tetradecanuclear Iron Nanocluster *Materials* **2011**, 4, 300-310.
- (4) W. Hermes, B. Chevalier, U. C. Rodewald, S. F. Matar, F. Weill, I. Schellenberg, R. Poettgen, H. Lueken, M. Speldrich; New Quaternary Hydride CeZnSnH<sub>1.5</sub>: Structure, Magnetism, and Chemical Bonding *Chemistry of Materials* **2011**, 23, 1096-1104.
- (5) F. Hussain, S. Sandriesser, M. Speldrich, G. R. Patzke; A new series of lanthanoid containing Keggin-type germanotungstates with acetate chelators:  $[Ln(CH_3COO)GeW_{11}O_{39}(H_2O)_2]^{12-}$  ( $Ln = Eu^{III}, Gd^{III}, Tb^{III}, Dy^{III}, Ho^{III}, Er^{III}, Tm^{III}$  and  $Yb^{III}$ ) *J. Solid State Chem.* **2011**, 184, 214-219.
- (6) M.-D. Serb, M. Speldrich, H. Lueken, U. Englert; Isomorphous Catena Transition Metal Squarates  $[M^{II}(C_4O_4)(dmsO)_2(OH_2)_2]$  ( $M = Co, Mn$ ) and Magnetic Investigation into their Solid Solution  $Co_xMn_{1-x}$  *Z. Anorg. Allg. Chem.* **2011**, 637, 536-542.
- (7) M. Speldrich, H. Schilder, H. Lueken, P. Kögerler; A Computational Framework for Magnetic Polyoxometalates and Molecular Spin Structures: CONDON 2.0 *Isr. J. Chem.* **2011**, 51, 215-227.
- (8) C. Ritchie, M. Speldrich, R. W. Gable, L. Sorace, P. Kögerler, C. Boskovic; Utilizing the Adaptive Polyoxometalate  $[As_2W_{19}O_{67}(H_2O)]^{14-}$  To Support a Polynuclear Lanthanoid-Based Single-Molecule Magnet *Inorg. Chem.* **2011**, 50, 7004-7014.
- (9) I. L. Malaestean, M. Speldrich, A. Ellern, S. G. Baca, P. Kögerler; Heterometal expansion of oxozirconium carboxylate clusters *Dalton Transactions* **2011**, 40, 331-333.

## Publikationen 2012

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- (1) I. L. Malaestean, M. Kutluca, M. Speldrich, A. Ellern, P. Kögerler; Macrocycles based on magnetically functionalized zirconium oxide clusters *Inorg. Chim. Acta* **2012**, 380, 72-77.
- (2) I. L. Malaestean, M. Kutluca-Alici, A. Ellern, J. van Leusen, H. Schilder, M. Speldrich, S. G. Baca, P. Kögerler; Linear, Zigzag, and Helical Cerium(III) Coordination Polymers, *Crystal Growth & Design* **2012**, 12, 1593-1602.
- (3) J. Fielden, M. Speldrich, C. Besson, P. Kögerler; Chiral Hexanuclear Ferric Wheels, *Inorg. Chem.* **2012**, 51, 2734-2736.
- (4) J. Fielden, D.-L. Long, M. Speldrich, P. Kögerler and L. Cronin;  $[Co_xCu_{1-x}(DDOP)(OH_2)(NO_3)](NO_3)$ : hydrogen bond-driven distortion of cobalt(II) by solid solution 'network mismatch', *Dalton Transactions* **2012**, 41, 4927-4934.
- (5) X. Fang , P. Kögerler , M. Speldrich , H. Schilder, M. Luban; A polyoxometalate-based single-molecule magnet with an  $S = 21/2$  ground state *Chem. Commun.* **2012**, 48, 1218-1220.
- (6) G. M. Dulcevscaia, I. G. Philippova, M. Speldrich, J. van Leusen, V. C. Kravtsov, S. G. Baca, P. Kögerler, S.-X. Liu, S. Decurtins; Cluster-Based Networks: 1D and 2D Coordination Polymers Based on  $MnFe_2(\mu_3-O)$ -Type Clusters, *Inorg. Chem.* **2012**, DOI.: 10.1021/ic202644t.
- (7) X. Tang, Manfred Speldrich, A. L. Tchougréeff, R. Dronskowski; Syntheses, Crystal Structures and Magnetic Properties of  $Cr(NCNH_2)_4Cl_2$  and  $Mn(NCNH_2)_4Cl_2$  *Z. Naturforsch. B* **2012**, submitted.
- (8) M. Kuiper, M. Speldrich, H. Schilder, H. Lueken; Magnetic Anisotropy of Dichlorobis( $\eta^5$ -cyclopentadienyl) Complexes of Vanadium, Niobium, and Tantalum, *Z. Anorg. Allg. Chem.* **2012**, submitted.

## Präsentationen

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08/2003	5th International Conference on f-elements (ICfe'5), Geneva, Switzerland; Titel: The valence state of uranium in $K_6Cu_{12}U_2S_{15}$
05/2007	Colloquium of SPP 1137 "Molekularer Magnetismus", Bad Dürkheim; Titel: Elucidation of the magnetic properties of $4f^7$ systems under consideration of zero field splitting, interatomic spin-spin coupling and applied magnetic field.
02/2009	Colloquium of SPP 1137 "Molekularer Magnetismus", Bad Dürkheim; Titel: Isomorphous Catena Transition Metal Squarates ( $M = Co(II), Mn(II)$ ) and magnetic investigation into their solid solutions ( $M = Co(II)_xMn(II)_{1-x}$ )
05/2009	XVI-th Conference "Physical Methods in Coordination and Supramolecular Chemistry", Chisinau, Republic of Moldova; Titel: A new heptanuclear iron(III) carboxylate cluster
07/2009	Vortrag beim Leverhulme Meeting 2009, Manchester, Großbritannien; Titel: Computational chemistry – The program CONDON –
12/2011	Vortrag an der Universität von Barcelona, Spanien; Titel: A Computational Framework for Molecular Spin Structures: CONDON 2.0

## EDV Kenntnisse

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Magnetochemie	Programm CONDON (Simulation von Molekularen Magneten) HTSE-Package (Magnetisch konzentrierter Systeme)
Betriebssysteme	UNIX (Linux, Solaris, etc.), Windows, MacOS
Sprachen	FORTRAN77, C/C++
Software	MS Office Anwendungen, Origin, CorelDraw Graphic Suite, ChemOffice, ISIS Draw, Sci-finder
Sonstiges	Grundkenntnisse im Bereich Hardware