Full list of publications
2018

Alexander Schnegg

1. Suturina, E. A.; Nehrkorn, J.; Zadrozny, J. M.; Liu, J.; Atanasov, M.; Weyhermüller, T.; Maganas, D.; Hill, S.; Schnegg, A.; Bill, E.; Long, J. R.; Neese, F., Magneto-Structural Correlations in Pseudotetrahedral Forms of the [Co(SPh)4]2– Complex Probed by Magnetometry, MCD Spectroscopy, Advanced EPR Techniques, and ab Initio Electronic Structure Calculations. *Inorganic Chemistry* **2017,** *56* (5), 3102-3118.
2. Schnegg, A., Very-High-Frequency EPR. In *eMagRes*, John Wiley & Sons, Ltd: 2017.
3. Palacios, M. A.; Nehrkorn, J.; Suturina, E. A.; Ruiz, E.; Gómez-Coca, S.; Holldack, K.; Schnegg, A.; Krzystek, J.; Moreno, J. M.; Colacio, E., Analysis of Magnetic Anisotropy and the Role of Magnetic Dilution in Triggering Single-Molecule Magnet (SMM) Behavior in a Family of CoIIYIII Dinuclear Complexes with Easy-Plane Anisotropy. *Chemistry – A European Journal* **2017,** *23* (48), 11649-11661.
4. Nehrkorn, J.; Veber, S.; Zhukas, L. A.; Novikov, V. V.; Nelyubina, Y.; Voloshin, Y. Z.; Holldack, K.; Stoll, S.; Schnegg, A., Determination of Large Temperature-Dependent Zero-Field Splitting in a High-Spin Co(I) Clathrochelate. *Inorganic Chemistry* **2017**.
5. Nehrkorn, J.; Holldack, K.; Bittl, R.; Schnegg, A., Recent progress in synchrotron-based frequency-domain Fourier-transform THz-EPR. *J. Magn. Reson.* **2017,** *280*, 10-19.
6. Möser, J.; Lips, K.; Tseytlin, M.; Eaton, G. R.; Eaton, S. S.; Schnegg, A., Using rapid-scan EPR to improve the detection limit of quantitative EPR by more than one order of magnitude. *J. Magn. Reson.* **2017,** *281*, 17-25.
7. Bucinsky, L.; Breza, M.; Lee, W.-T.; Hickey, A. K.; Dickie, D. A.; Nieto, I.; DeGayner, J. A.; Harris, T. D.; Meyer, K.; Krzystek, J.; Ozarowski, A.; Nehrkorn, J.; Schnegg, A.; Holldack, K.; Herber, R. H.; Telser, J.; Smith, J. M., Spectroscopic and Computational Studies of Spin States of Iron(IV) Nitrido and Imido Complexes. *Inorganic Chemistry* **2017,** *56* (8), 4751-4768.
8. Schnegg, A.; Nehrkorn, J.; Singh, A.; Calafell, I. A.; Bonke, S. A.; Hocking, R. K.; Lips, K.; Spiccia, L., Probing the Fate of Mn Complexes in Nafion: A Combined Multifrequency EPR and XAS Study. *The Journal of Physical Chemistry C* **2016,** *120* (2), 853-861.
9. Jia, H.; Roa, R.; Angioletti-Uberti, S.; Henzler, K.; Ott, A.; Lin, X.; Möser, J.; Kochovski, Z.; Schnegg, A.; Dzubiella, J., Thermosensitive Cu 2 O–PNIPAM core–shell nanoreactors with tunable photocatalytic activity. *Journal of Materials Chemistry A* **2016,** *4* (24), 9677-9684.
10. Holldack, K.; Schnegg, A., THz Electron Paramagnetic Resonance/THz Spectroscopy at BESSY II. *Journal of large-scale research facilities JLSRF* **2016,** *2*, 51.
11. Feng, X.; Liu, J.-L.; Pedersen, K. S.; Nehrkorn, J.; Schnegg, A.; Holldack, K.; Bendix, J.; Sigrist, M.; Mutka, H.; Samohvalov, D., Multifaceted magnetization dynamics in the mononuclear complex [Re IV Cl 4 (CN) 2] 2−. *Chemical Communications* **2016,** *52* (87), 12905-12908.
12. Bragaglia, V.; Schnegg, A.; Calarco, R.; Holldack, K., Epitaxial Ge2Sb2Te5 probed by single cycle THz pulses of coherent synchrotron radiation. *Appl. Phys. Lett.* **2016,** *109* (14), 141903.
13. Astakhov, O.; Xiao, L.; Finger, F.; Chen, T.; Fehr, M.; George, B.; Schnegg, A.; Lips, K.; Teutloff, C., Multifrequency EPR study of HWCVD μc-SiC: H for photovoltaic applications. *physica status solidi (a)* **2016**.
14. Sallmann, M.; Kumar, S.; Chernev, P.; Nehrkorn, J.; Schnegg, A.; Kumar, D.; Dau, H.; Limberg, C.; de Visser, S. P., Structure and mechanism leading to formation of the cysteine sulfinate product complex of a biomimetic cysteine dioxygenase model. *Chemistry–A European Journal* **2015,** *21* (20), 7470-7479.

15. Pinkowicz, D.; Southerland, H. I.; Avendaño, C.; Prosvirin, A.; Sanders, C.; Wernsdorfer, W.; Pedersen, K. S.; Dreiser, J.; Clérac, R.; Nehrkorn, J.; Simeoni, G. G.; Schnegg, A.; Holldack, K.; Dunbar, K. R., Cyanide Single-Molecule Magnets Exhibiting Solvent Dependent Reversible "On" and "Off" Exchange Bias Behavior. *Journal of the American Chemical Society* **2015,** *137* (45), 14406-14422.
16. Nehrkorn, J.; Telser, J.; Holldack, K.; Stoll, S.; Schnegg, A., Simulating frequency-domain electron paramagnetic resonance: Bridging the gap between experiment and magnetic parameters for high-spin transition-metal ion complexes. *The Journal of Physical Chemistry B* **2015,** *119* (43), 13816-13824.
17. Nehrkorn, J.; Schnegg, A.; Holldack, K.; Stoll, S., General Magnetic Transition Dipole Moments for Electron Paramagnetic Resonance. *Physical review letters* **2015,** *114* (1), 010801.
18. Melskens, J.; Schnegg, A.; Baldansuren, A.; Lips, K.; Plokker, M.; Eijt, S.; Schut, H.; Fischer, M.; Zeman, M.; Smets, A., Structural and electrical properties of metastable defects in hydrogenated amorphous silicon. *Physical Review B* **2015,** *91* (24), 245207.
19. Katz, I.; Fehr, M.; Schnegg, A.; Lips, K.; Blank, A., High resolution in-operando microimaging of solar cells with pulsed electrically-detected magnetic resonance. *J. Magn. Reson.* **2015,** *251*, 26-35.
20. Akhtar, W.; Schnegg, A.; Veber, S.; Meier, C.; Fehr, M.; Lips, K., CW and pulsed electrically detected magnetic resonance spectroscopy at 263GHz/12T on operating amorphous silicon solar cells. *J. Magn. Reson.* **2015,** *257*, 94-101.
21. Steffens, S.; Becker, C.; Amkreutz, D.; Klossek, A.; Kittler, M.; Chen, Y.-Y.; Schnegg, A.; Klingsporn, M.; Abou-Ras, D.; Lips, K., Impact of dislocations and dangling bond defects on the electrical performance of crystalline silicon thin films. *Appl. Phys. Lett.* **2014,** *105* (2), 022108.
22. Ling, Y.; Van Mierloo, S.; Schnegg, A.; Fehr, M.; Adriaensens, P.; Lutsen, L.; Vanderzande, D.; Maes, W.; Goovaerts, E.; Van Doorslaer, S., Electronic structure of positive and negative polarons in functionalized dithienylthiazolo [5, 4-d] thiazoles: a combined EPR and DFT study. *Phys Chem Chem Phys* **2014,** *16* (21), 10032-10040.
23. Fehr, M.; Schnegg, A.; Rech, B.; Astakhov, O.; Finger, F.; Bittl, R.; Teutloff, C.; Lips, K., Metastable Defect Formation at Microvoids Identified as a Source of Light-Induced Degradation in a− Si: H. *Physical review letters* **2014,** *112* (6), 066403.
24. Sontheimer, T.; Schnegg, A.; Steffens, S.; Ruske, F.; Amkreutz, D.; Lips, K.; Rech, B., Identification of intra-grain and grain boundary defects in polycrystalline Si thin films by electron paramagnetic resonance. *physica status solidi (RRL)-Rapid Research Letters* **2013,** *7* (11), 959-962.
25. Sontheimer, T.; Preidel, V.; Lockau, D.; Back, F.; Rudigier-Voigt, E.; Löchel, B.; Erko, A.; Schmidt, F.; Schnegg, A.; Lips, K., Correlation between structural and opto-electronic characteristics of crystalline Si microhole arrays for photonic light management. *Journal of Applied Physics* **2013,** *114* (17), 173513.
26. Singh, A.; Hocking, R. K.; Chang, S. L.-Y.; George, B. M.; Fehr, M.; Lips, K.; Schnegg, A.; Spiccia, L., Water oxidation catalysis by nanoparticulate manganese oxide thin films: probing the effect of the manganese precursors. *Chem. Mat.* **2013,** *25* (7), 1098-1108.
27. Nehrkorn, J.; Martins, B. M.; Holldack, K.; Stoll, S.; Dobbek, H.; Bittl, R.; Schnegg, A., Zero-field splittings in metHb and metMb with aquo and fluoro ligands: a FD-FT THz-EPR study. *Mol. Phys.* **2013,** *111* (18-19), 2696-2707.
28. Mitchell, D. G.; Tseitlin, M.; Quine, R. W.; Meyer, V.; Newton, M. E.; Schnegg, A.; George, B.; Eaton, S. S.; Eaton, G. R., X-band rapid-scan EPR of samples with long electron spin relaxation times: a comparison of continuous wave, pulse and rapid-scan EPR. *Mol. Phys.* **2013,** *111* (18-19), 2664-2673.
29. Meier, C.; Behrends, J.; Teutloff, C.; Astakhov, O.; Schnegg, A.; Lips, K.; Bittl, R., Multi-frequency EDMR applied to microcrystalline thin-film silicon solar cells. *J. Magn. Reson.* **2013,** *234*, 1-9.

30. George, B.; Behrends, J.; Schnegg, A.; Schulze, T.; Fehr, M.; Korte, L.; Rech, B.; Lips, K.; Rohrmüller, M.; Rauls, E., Atomic structure of interface states in silicon heterojunction solar cells. *Physical review letters* **2013,** *110* (13), 136803.
31. Dreiser, J.; Pedersen, K. S.; Schnegg, A.; Holldack, K.; Nehrkorn, J.; Sigrist, M.; Tregenna-Piggott, P.; Mutka, H.; Weihe, H.; Mironov, V. S., Three-Axis Anisotropic Exchange Coupling in the Single-Molecule Magnets NEt4 [MnIII2 (5-Brsalen) 2 (MeOH) 2MIII (CN) 6](M= Ru, Os). *Chem.-Eur. J.* **2013,** *19* (11), 3693-3701.
32. Dikarov, E.; Fehr, M.; Schnegg, A.; Lips, K.; Blank, A., Selective electron spin resonance measurements of micrometer-scale thin samples on a substrate. *Measurement Science and Technology* **2013,** *24* (11), 115009.
33. Behrends, J.; Samuel, I. D.; Schnegg, A.; Keeble, D. J., Persistent spin coherence and bipolarons. *Nature nanotechnology* **2013,** *8* (12), 884-885.
34. Schnegg, A.; Behrends, J.; Fehr, M.; Lips, K., Pulsed electrically detected magnetic resonance for thin film silicon and organic solar cells. *Phys Chem Chem Phys* **2012,** *14* (42), 14418-14438.
35. Salzmann, I.; Heimel, G.; Duhm, S.; Oehzelt, M.; Pingel, P.; George, B. M.; Schnegg, A.; Lips, K.; Blum, R.-P.; Vollmer, A., Intermolecular hybridization governs molecular electrical doping. *Physical review letters* **2012,** *108* (3), 035502.
36. Hoehne, F.; Dreher, L.; Behrends, J.; Fehr, M.; Huebl, H.; Lips, K.; Schnegg, A.; Suckert, M.; Stutzmann, M.; Brandt, M. S., Lock-in detection for pulsed electrically detected magnetic resonance. *Review of Scientific Instruments* **2012,** *83* (4), 043907.
37. Forshaw, A. P.; Smith, J. M.; Ozarowski, A.; Krzystek, J.; Smirnov, D.; Zvyagin, S.; Harris, T. D.; Karunadasa, H. I.; Zadrozny, J. M.; Schnegg, A., Low-spin hexacoordinate Mn (III): synthesis and spectroscopic investigation of homoleptic tris (pyrazolyl) borate and tris (carbene) borate complexes. *Inorganic chemistry* **2012,** *52* (1), 144-159.
38. Fehr, M.; Simon, P.; Sontheimer, T.; Leendertz, C.; Gorka, B.; Schnegg, A.; Rech, B.; Lips, K., Influence of deep defects on device performance of thin-film polycrystalline silicon solar cells. *Appl. Phys. Lett.* **2012,** *101* (12), 123904.
39. Fehr, M.; Schnegg, A.; Rech, B.; Lips, K.; Astakhov, O.; Finger, F.; Freysoldt, C.; Bittl, R.; Teutloff, C., Dangling bonds in amorphous silicon investigated by multifrequency EPR. *J. Non-Cryst. Solids* **2012,** *358* (17), 2067-2070.
40. Behrends, J.; Sperlich, A.; Schnegg, A.; Biskup, T.; Teutloff, C.; Lips, K.; Dyakonov, V.; Bittl, R., Direct detection of photoinduced charge transfer complexes in polymer fullerene blends. *Physical Review B* **2012,** *85* (12), 125206.
41. Pedersen, K. S.; Dreiser, J.; Nehrkorn, J.; Gysler, M.; Schau-Magnussen, M.; Schnegg, A.; Holldack, K.; Bittl, R.; Piligkos, S.; Weihe, H., A linear single-molecule magnet based on [Ru III (CN) 6] 3−. *Chemical Communications* **2011,** *47* (24), 6918-6920.
42. Muhrer, G.; Hartl, M.; Daemen, L.; Tovesson, F.; Schnegg, A.; Russina, M.; Schachinger, E., Scattering law of a magnesium hydride moderator. *Nuclear Instruments and Methods in Physics Research Section A: Accelerators, Spectrometers, Detectors and Associated Equipment* **2011,** *629* (1), 251-259.
43. Fehr, M.; Schnegg, A.; Rech, B.; Lips, K.; Astakhov, O.; Finger, F.; Pfanner, G.; Freysoldt, C.; Neugebauer, J.; Bittl, R., Combined multifrequency EPR and DFT study of dangling bonds in a-Si: H. *Physical Review B* **2011,** *84* (24), 245203.
44. Fehr, M.; Behrends, J.; Haas, S.; Rech, B.; Lips, K.; Schnegg, A., Electrical detection of electron-spin-echo envelope modulations in thin-film silicon solar cells. *Physical Review B* **2011,** *84* (19), 193202.
45. Dreiser, J.; Schnegg, A.; Holldack, K.; Pedersen, K. S.; Schau-Magnussen, M.; Nehrkorn, J.; Tregenna-Piggott, P.; Mutka, H.; Weihe, H.; Bendix, J., Frequency-Domain Fourier-Transform Terahertz Spectroscopy of the Single-Molecule Magnet (NEt4)[Mn2 (5-Brsalen) 2 (MeOH) 2Cr (CN) 6]. *Chemistry–A European Journal* **2011,** *17* (27), 7492-7498.

46. Fehr, M.; Schnegg, A.; Teutloff, C.; Bittl, R.; Astakhov, O.; Finger, F.; Rech, B.; Lips, K., Hydrogen distribution in the vicinity of dangling bonds in hydrogenated amorphous silicon (a-Si: H). *physica status solidi (a)* **2010,** *207* (3), 552-555.
47. Bordignon, E.; Brutlach, H.; Urban, L.; Hideg, K.; Savitsky, A.; Schnegg, A.; Gast, P.; Engelhard, M.; Groenen, E.; Möbius, K., Heterogeneity in the nitroxide micro-environment: polarity and proticity effects in spin-labeled proteins studied by multi-frequency EPR. *Appl. Magn. Reson.* **2010,** *37* (1-4), 391.
48. Behrends, J.; Schnegg, A.; Lips, K.; Thomsen, E.; Pandey, A.; Samuel, I.; Keeble, D., Bipolaron formation in organic solar cells observed by pulsed electrically detected magnetic resonance. *Physical review letters* **2010,** *105* (17), 176601.
49. Schnegg, A.; Behrends, J.; Lips, K.; Bittl, R.; Holldack, K., Frequency domain Fourier transform THz-EPR on single molecule magnets using coherent synchrotron radiation. *Phys Chem Chem Phys* **2009,** *11* (31), 6820-6825.
50. Behrends, J.; Schnegg, A.; Fehr, M.; Lambertz, A.; Haas, S.; Finger, F.; Rech, B.; Lips, K., Electrical detection of electron spin resonance in microcrystalline silicon pin solar cells. *Philos. Mag.* **2009,** *89* (28-30), 2655-2676.
51. Bagryanskaya, E. G.; Polovyanenko, D. N.; Fedin, M. V.; Kulik, L.; Schnegg, A.; Savitsky, A.; Möbius, K.; Coleman, A. W.; Ananchenko, G. S.; Ripmeester, J. A., Multifrequency EPR study of the mobility of nitroxides in solid-state calixarene nanocapsules. *Phys Chem Chem Phys* **2009,** *11* (31), 6700-6707.
52. Polovyanenko, D. N.; Bagryanskaya, E. G.; Schnegg, A.; Möbius, K.; Coleman, A. W.; Ananchenko, G. S.; Udachin, K. A.; Ripmeester, J. A., Inclusion of 4-methoxy-2, 2, 6, 6-tetramethylpiperidine-N-oxyl in a calixarene nanocapsule in the solid state. *Phys Chem Chem Phys* **2008,** *10* (34), 5299-5307.
53. Okafuji, A.; Schnegg, A.; Schleicher, E.; Möbius, K.; Weber, S., G-Tensors of the Flavin Adenine Dinucleotide Radicals in Glucose Oxidase: A Comparative Multifrequency Electron Paramagnetic Resonance and Electron− Nuclear Double Resonance Study. *The Journal of Physical Chemistry B* **2008,** *112* (11), 3568-3574.
54. Behrends, J.; Schnegg, A.; Boehme, C.; Haas, S.; Stiebig, H.; Finger, F.; Rech, B.; Lips, K., Recombination and transport in microcrystalline pin solar cells studied with pulsed electrically detected magnetic resonance. *J. Non-Cryst. Solids* **2008,** *354* (19), 2411-2415.
55. Schnegg, A.; Dubinskii, A.; Fuchs, M.; Grishin, Y. A.; Kirilina, E.; Lubitz, W.; Plato, M.; Savitsky, A.; Möbius, K., High-field EPR, ENDOR and ELDOR on bacterial photosynthetic reaction centers. *Appl. Magn. Reson.* **2007,** *31* (1-2), 59-98.
56. Schnegg, A.; Okafuji, A.; Bacher, A.; Bittl, R.; Fischer, M.; Fuchs, M.; Hegemann, P.; Joshi, M.; Kay, C.; Richter, G., Towards an identification of chemically different flavin radicals by means of theirg-tensor. *Appl. Magn. Reson.* **2006,** *30* (3-4), 345-358.
57. Schnegg, A.; Kay, C.; Schleicher, E.; Hitomi, K.; Todo, T.; Möbius, K.; Weber∗, S., The g-tensor of the flavin cofactor in (6–4) photolyase: a 360 GHz/12.8 T electron paramagnetic resonance study. *Mol. Phys.* **2006,** *104* (10-11), 1627-1633.
58. Mobius, K.; Schnegg, A.; Plato, M.; Fuchs, M.; Savitsky, A., High-field EPR spectroscopy on transfer proteins in biological action. *ACTA PHYSICA POLONICA SERIES A* **2005,** *108* (2), 215.
59. Möbius, K.; Savitsky, A.; Wegener, C.; Plato, M.; Fuchs, M.; Schnegg, A.; Dubinskii, A.; Grishin, Y. A.; Grigor'ev, I.; Kühn, M., Combining high-field EPR with site-directed spin labeling reveals unique information on proteins in action. *Magn. Reson. Chem.* **2005,** *43* (S1), S4-S19.
60. Möbius, K.; Savitsky, A.; Schnegg, A.; Plato, M.; Fuchs, M., High-field EPR spectroscopy applied to biological systems: characterization of molecular switches for electron and ion transfer. *Phys Chem Chem Phys* **2005,** *7* (1), 19-42.
61. Kirilina, E. P.; Prisner, T. F.; Bennati, M.; Endeward, B.; Dzuba, S. A.; Fuchs, M. R.; Möbius, K.; Schnegg, A., Molecular dynamics of nitroxides in glasses as studied by multi-frequency EPR. *Magn. Reson. Chem.* **2005,** *43* (S1).

62. Grishin, Y. A.; Fuchs, M.; Schnegg, A.; Dubinskii, A.; Dumesh, B.; Rusin, F.; Bratman, V.; Möbius, K., Pulsed Orotron—A new microwave source for submillimeter pulse high-field electron paramagnetic resonance spectroscopy. *Review of Scientific Instruments* **2004,** *75* (9), 2926-2936.
63. Fuchs, M. R.; Schnegg, A.; Plato, M.; Schulz, C.; Müh, F.; Lubitz, W.; Möbius, K., The primary donor cation P+ in photosynthetic reaction centers of site-directed mutants of Rhodobacter sphaeroides: g-tensor shifts revealed by high-field EPR at 360 GHz/12.8 T. *Chemical physics* **2003,** *294* (3), 371-384.
64. Carmieli, R.; Manikandan, P.; Epel, B.; Kalb, A. J.; Schnegg, A.; Savitsky, A.; Mobius, K.; Goldfarb, D., Dynamics in the Mn2+ binding site in single crystals of concanavalin A revealed by high-field EPR spectroscopy. *BIOCHEMISTRY-PENNSYLVANIA THEN WASHINGTON-* **2003,** *42* (25), 7863-7870.
65. Schnegg, A.; Fuhs, M.; Rohrer, M.; Lubitz, W.; Prisner, T.; Möbius, K., Molecular dynamics of QA-• and QB-• in photosynthetic bacterial reaction centers studied by pulsed high-field EPR at 95 GHz. *The Journal of Physical Chemistry B* **2002,** *106* (36), 9454-9462.
66. Fuhs, M.; Schnegg, A.; Prisner, T.; Köhne, I.; Hanley, J.; Rutherford, A.; Möbius, K., Orientation selection in photosynthetic PS I multilayers: structural investigation of the charge separated state P 700+ A 1− by high-field/high-frequency time-resolved EPR at 3.4 T/95 GHz. *Biochimica et Biophysica Acta (BBA)-Bioenergetics* **2002,** *1556* (1), 81-88.
67. Fuchs, M. R.; Schleicher, E.; Schnegg, A.; Kay, C. W.; Törring, J. T.; Bittl, R.; Bacher, A.; Richter, G.; Möbius, K.; Weber, S., g-Tensor of the neutral flavin radical cofactor of DNA photolyase revealed by 360-GHz electron paramagnetic resonance spectroscopy. *The Journal of Physical Chemistry B* **2002,** *106* (34), 8885-8890.