

## List of publications: Dr. Alexander Schnegg

### 2020

- Pavlov, A.A., Nehr Korn, J., Zubkevich, S.V., Fedin, M.V., Holldack, K., **Schnegg, A.**, Novikov, V.V. (2020). A Synergy and Struggle of EPR, Magnetometry and NMR: A Case Study of Magnetic Interaction Parameters in a Six-Coordinate Cobalt(II) Complex *Inorganic Chemistry* 59(15), 10746-10755. <https://doi.org/10.1021/acs.inorgchem.0c01191>
- Viciano-Chumillas, M., Blondin, G., Clémanceym N., Krzystek, J., Ozerov, M., Armentano, D., **Schnegg, A.**, Lohmiller, T., Telsler, J., Lloret, F., Cano, J. (2020). Single-Ion Magnetic Behaviour in an Iron(III) Porphyrin Complex: A Dichotomy Between High-Spin and 5/2–3/2 Spin Admixture *Chemistry – A European Journal* <https://doi.org/10.1002/chem.202003052>
- Jochim, A., Lohmiller, T., Rams, M., Böhme, M., Ceglarska, M., **Schnegg, A.**, Plass, W., Näther, C. (2020). Influence of the Coligand onto the Magnetic Anisotropy and the Magnetic Behavior of One-Dimensional Coordination Polymers *Inorganic Chemistry* 59(13), 8971-8982. <https://doi.org/10.1021/acs.inorgchem.0c00815>
- Lin, Y.-H., Kutin, Y., van Gastel, M., Bill, E., **Schnegg, A.**, Ye, S., Lee, W.-Z. (2020). A Manganese(IV)-Hydroperoxo Intermediate Generated by Protonation of the Corresponding Manganese(III)-Superoxo Complex *Journal of the American Chemical Society* 142(23), 10255-10260. <https://doi.org/10.1021/jacs.0c02756>
- Böhme, M., Jochim, A., Rams, M., Lohmiller, T., Suckert, S., **Schnegg, A.**, Plass, W., Näther, C. (2020). Variation of the Chain Geometry in Isomeric 1D Co(NCS)<sub>2</sub> Coordination Polymers and Their Influence on the Magnetic Properties *Inorganic Chemistry* 59(8), 5325-5338. <https://doi.org/10.1021/acs.inorgchem.9b03357>
- Ma, Y., Pang, Y., Chabbra, S., Reijerse, E.J., **Schnegg, A.**, Niski, J., Leutzsch, M., Cornella, J. (2020). Radical C–N Borylation of Aromatic Amines Enabled by a Pyrylium Reagent *Chemistry – A European Journal* 26(17), 3734-3743. <https://doi.org/10.1002/chem.202000412>
- Krzystek, J., **Schnegg, A.**, Aliabadi, A., Holldack, K., Stoian, S.A., Ozarowski, A., Hicks, S.D., Abu-Omar, M.M., Thomas, K.E., Ghosh, A., Caulfield, K.P., Tonzetich, Z.J., Telsler, J. (2020). Advanced Paramagnetic Resonance Studies on Manganese and Iron Corroles with a Formal d<sup>4</sup> Electron Count *Inorganic Chemistry* 59(2), 1075-1090. <https://doi.org/10.1021/acs.inorgchem.9b02635>
- Li, J., Chen, J., Sang, R., Ham, W.-S., Plutschack, M.B., Berger, F., Chabbra, S., **Schnegg, A.**, Genicot, C., Ritter, T. (2020). Photoredox catalysis with aryl sulfonium salts enables site-selective late-stage fluorination *Nature Chemistry* 12, 56-62. <https://doi.org/10.1038/s41557-019-0353-3>
- Rams, M., Jochim, A., Böhme, M., Lohmiller, T., Ceglarska, M., Rams, M.M., **Schnegg, A.**, Plass, W., Näther, C. (2020). Single-Chain Magnet Based on Cobalt(II) Thiocyanate as XXZ Spin Chain *Chemistry – A European Journal* 26(13), 2837-2851. <https://doi.org/10.1002/chem.201903924>

### 2019

- Kutin, Y., Cox, N., Lubitz, W., **Schnegg, A.**, Rüdiger, O. (2019). In Situ EPR Characterization of a Cobalt Oxide Water Oxidation Catalyst at Neutral pH *Catalysts* 9(11), 926. <https://doi.org/10.3390/catal9110926>

- Nehr Korn, J., Bonke, S.A., Aliabadi, A., Schwalbe, M., **Schnegg, A.** (2019). Examination of the Magneto-Structural Effects of Hangman Groups on Ferric Porphyrins by EPR *Inorganic Chemistry* 58(20), 14228-14237. <https://doi.org/10.1021/acs.inorgchem.9b02348>
- Sidabras, J., Duan, J., Winkler, M., Happe, T., Hussein, R., Zouni, A., Suter, D., **Schnegg, A.**, Lubitz, W., Reijerse, E.J. (2019) Extending electron paramagnetic resonance to nanoliter volume protein single crystals using a self-resonant microhelix *Science Advances* 5(10), eaay1394. <https://doi.org/10.1126/sciadv.aay1394>
- Cheng, J., Liu, J., Leng, X., Lohmiller, T., **Schnegg, A.**, Bill, E., Ye, S., Deng, L. (2019). A Two-Coordinate Iron(II) Imido Complex with NHC Ligation: Synthesis, Characterization, and Its Diversified Reactivity of Nitrene Transfer and C–H Bond Activation *Inorganic Chemistry* 58, 7634-7644. <https://doi.org/10.1021/acs.inorgchem.9b01147>
- Zhao, G., Busser, G.W., Froese, C., Hu, B., Bohnke, S.A., **Schnegg, A.**, Ai, Y., Wei, D., Wang, X., Peng, B., Muhler, M. (2019). Anaerobic Alcohol Conversion to Carbonyl Compounds Over Nanoscaled Rh-doped SrTiO<sub>3</sub> under Visible Light *The Journal of Physical Chemistry Letters* 10, 2075–2080. <https://doi.org/10.1021/acs.jpcclett.9b00621>

## 2018

- Nehr Korn, J., Veber, S.L., Zhukas, L.A., Novikov, V.N., Nelyubina, Y.V., Voloshin, Y.Z., Holldack, K., Stoll, S., **Schnegg, A.** (2018). Determination of Large Zero-Field Splitting in High-Spin Co(I) Clathrochelates *Inorganic Chemistry* 57(24), 15330-15340. <https://doi.org/10.1021/acs.inorgchem.8b02670>
- Riedel, W., Thum, L., Moser, J., Fleischer, V., Simon, U., Siemensmeyer, K., **Schnegg, A.**, Schomacker, R., Risse, T., Dinse, K.P. (2018). Magnetic Properties of Reduced and Reoxidized Mn-Na<sub>2</sub>WO<sub>4</sub>/SiO<sub>2</sub>: A Catalyst for Oxidative Coupling of Methane (OCM) *Journal of Physical Chemistry C* 122(39), 22605-22614. <https://doi.org/10.1021/acs.jpcc.8b07386>
- Böhme, M., Ziegenbalg, S., Aliabadi, A., **Schnegg, A.**, Górls, H., Plass, W. (2018). Magnetic relaxation in cobalt(II)-based single-ion magnets influenced by distortion of the pseudotetrahedral [N<sub>2</sub>O<sub>2</sub>] coordination environment *Dalton Transactions* 47(32), 10861-10873. <https://doi.org/10.1039/c8dt01530a>

## 2017

- Palacios, M.A., Nehr Korn, J., Suturina, E.A., Ruiz, E., Gómez-Coca, S., Holldack, K., **Schnegg, A.**, Krzystek, J., Moreno, J.M., Colacio, E. (2017). Analysis of Magnetic Anisotropy and the Role of Magnetic Dilution in Triggering Single-Molecule Magnet (SMM) Behavior in a Family of Co<sup>II</sup>Y<sup>III</sup> Dinuclear Complexes with Easy-Plane Anisotropy *Chemistry - A European Journal* 23(48), 11649-11661. <https://doi.org/10.1002/chem.201702099>
- Möser, J., Lips, K., Tseytlin, M., Eaton, G.R., Eaton, S.S., **Schnegg, A.** (2017). Using rapid-scan EPR to improve the detection limit of quantitative EPR by more than one order of magnitude *Journal of Magnetic Resonance* 281, 17-25. <https://doi.org/10.1016/j.jmr.2017.04.003>
- Nehr Korn, J., Holldack, K., Bittl, R., **Schnegg, A.** (2017). Recent progress in synchrotron-based frequency-domain Fourier-transform THz-EPR *Journal of Magnetic Resonance* 280, 10-19. <https://doi.org/10.1016/j.jmr.2017.04.001>

- 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., Nehr Korn, J., **Schnegg, A.**, Holldack, K., Herber, R.H., Telser, J., Smith, J.M. (2017). Spectroscopic and Computational Studies of Spin States of Iron(IV) Nitrido and Imido Complexes *Inorganic Chemistry* 56(8), 4751-4768. <https://doi.org/10.1021/acs.inorgchem.7b00512>
- Suturina, E.A., Nehr Korn, J., Zadrozny, J.M., Liu, J., Atanasov, M., Weyhermüller, T., Maganas, D., Hill, S., **Schnegg, A.**, Bill, E., Long, J.R., Neese, F. (2017). Magneto-Structural Correlations in Pseudotetrahedral Forms of the  $[\text{Co}(\text{SPh})_4]^{2-}$  Complex Probed by Magnetometry, MCD Spectroscopy, Advanced EPR Techniques, and ab Initio Electronic Structure Calculations *Inorganic Chemistry* 56(5), 3102-3118. <https://doi.org/10.1021/acs.inorgchem.7b00097>
- **Schnegg, A.** (2017). Very-high-frequency EPR *eMagRes* 6 (1), 115-131. <https://doi.org/10.1002/9780470034590.emrstm1526>

## 2016

- Holldack, K., **Schnegg, A.** (2016). THz Electron Paramagnetic Resonance / THz Spectroscopy at BESSY II *Journal of large-scale research facilities JLSRF* 2, A51. <https://doi.org/10.17815/jlsrf-2-74>
- Bragaglia, V., **Schnegg, A.**, Calarco, R., Holldack, K. (2016). Epitaxial  $\text{Ge}_2\text{Sb}_2\text{Te}_5$  probed by single cycle THz pulses of coherent synchrotron radiation *Applied Physics Letters* 109(14), 141903. <https://doi.org/10.1063/1.4963889>
- Astakhov, O., Xiao, L.H., Finger, F., Chen, T., Fehr, M., George, B., **Schnegg, A.**, Lips, K., Teutloff, C. (2016). Multifrequency EPR study of HWCVD  $\mu\text{-SiC:H}$  for photovoltaic applications *Physica Status Solidi A - Applications And Materials Science* 213(7), 1747-1750. <https://doi.org/10.1002/pssa.201533027>
- **Schnegg, A.**, Nehr Korn, J., Singh, A., Calafell, I.A., Bonke, S.A., Hocking, R.K., Lips, K., Spiccia, L. (2016). Probing the Fate of Mn Complexes in Nafion: A Combined Multifrequency EPR and XAS Study *Journal of Physical Chemistry C* 120(2), 853-861. <https://doi.org/10.1021/acs.jpcc.5b10451>
- Jia, H., Roa, R., Angioletti-Uberti, S., Henzler, K., Ott, A., Lin, X.Z., Möser, J., Kochovski, Z., **Schnegg, A.**, Dzubiella, J., Ballauff, M., Lu, Y. (2016). Thermosensitive  $\text{Cu}_2\text{O}$ -PNIPAM core-shell nanoreactors with tunable photocatalytic activity *Journal of Materials Chemistry A* 4(24), 9677-9684. <https://doi.org/10.1039/c6ta03528k>
- Feng, X., Liu, J.-L., Pedersen, K.S., Nehr Korn, J., **Schnegg, A.**, Holldack, K., Bendix, J., Sigrist, M., Mutka, H., Samohvalov, D., Aguilà, D., Tong, M.-L., Long, J.R., Clérac, R. (2016). Multifaceted magnetization dynamics in the mononuclear complex  $[\text{Re}^{\text{IV}}\text{Cl}_4(\text{CN})_2]^{2-}$  *Chemical Communications* 52(87), 12905-12908. <https://doi.org/10.1039/c6cc05473k>

## 2015

- Pinkowicz, D., Southerland, H.I., Avendano, C., Prosvirin, A., Sanders, C., Wernsdorfer, W., Pedersen, K.S., Dreiser, J., Clérac, R., Nehr Korn, J., Simeoni, G.G., **Schnegg, A.**, Holldack, K., Dunbar, K.R. (2015). Cyanide Single-Molecule Magnets Exhibiting Solvent Dependent Reversible "On" and "Off" Exchange Bias Behavior *Journal of the American Chemical Society* 137(45), 14406-14422. <https://doi.org/10.1021/jacs.5b09378>

- Nehr Korn, J., Telser, J., Holldack, K., Stoll, S., **Schnegg, A.** (2015). Simulating Frequency-Domain Electron Paramagnetic Resonance: Bridging the Gap between Experiment and Magnetic Parameters for High-Spin Transition-Metal Ion Complexes *Journal of Physical Chemistry B* 119(43), 13816-13824. <https://doi.org/10.1021/acs.jpcc.5b04156>
- Akhtar, W., **Schnegg, A.**, Veber, S., Meier, C., Fehr, M., Lips, K. (2015). CW and pulsed electrically detected magnetic resonance spectroscopy at 263 GHz/12T on operating amorphous silicon solar cells *Journal of Magnetic Resonance* 257, 94-101. <https://doi.org/10.1016/j.jmr.2015.05.012>
- Melskens, J., **Schnegg, A.**, Baldansuren, A., Lips, K., Plokker, M.P., Eijt, S.W.H., Schut, H., Fischer, M., Zeman, M., Smets, A.H.M. (2015). Structural and electrical properties of metastable defects in hydrogenated amorphous silicon *Physical Review B* 91(24), 245207. <https://doi.org/10.1103/PhysRevB.91.245207>
- Sallmann, M., Kumar, S., Chernev, P., Nehr Korn, J., **Schnegg, A.**, Kumar, D., Dau, H., Limberg, C., de Visser, S.P. (2015). Structure and Mechanism Leading to Formation of the Cysteine Sulfinate Product Complex of a Biomimetic Cysteine Dioxygenase Model *Chemistry – A European Journal* 21(20), 7470-7479. <https://doi.org/10.1002/chem.201500644>
- Katz, I., Fehr, M., **Schnegg, A.**, Lips, K., Blank, A. (2015). High-resolution *in-operando* microimaging of solar cells with pulsed electrically-detected magnetic resonance *Journal of Magnetic Resonance* 251, 26-35. <https://doi.org/10.1016/j.jmr.2014.11.008>
- Nehr Korn, J., **Schnegg, A.**, Holldack, K., Stoll, S. (2015). General Magnetic Transition Dipole Moments for Electron Paramagnetic Resonance *Physical Review Letters* 114(1), 10801. <https://doi.org/10.1103/PhysRevLett.114.010801>

## 2014

- Steffens, S., Becker, C., Amkreutz, D., Klossek, A., Kittler, M., Chen, Y.-Y., **Schnegg, A.**, Klingsporn, M., Abou-Ras, D., Lips, K., Rech, B. (2014). Impact of dislocations and dangling bond defects on the electrical performance of crystalline silicon thin films *Journal of Physical Chemistry Letters* 105(2), 22108. <https://doi.org/10.1063/1.4890625>
- Sontheimer, T., Amkreutz, D., Schulz, K., Wobkenberg, P.H., Guenther, C., Bakumov, V., Erz, J., Mader, C., Traut, S., Ruske, F., Weizman, M., **Schnegg, A.**, Patz, M., Trocha, M., Wunnicke, O., Rech, B. (2014). Solution-Processed Crystalline Silicon Thin-Film Solar Cells *Advanced Materials Interfaces* 1(3), 1300046. <https://doi.org/10.1002/admi.201300046>
- Fehr, M., **Schnegg, A.**, Rech, B., Astakhov, O., Finger, F., Bittl, R., Teutloff, C., Lips, K. (2014). Metastable Defect Formation at Microvoids Identified as a Source of Light-Induced Degradation in  $\alpha$ -Si:H *Physical Review Letters* 112(6), 66403. <https://doi.org/10.1103/PhysRevLett.112.066403>
- Ling, Y., Van Mierloo, S., **Schnegg, A.**, Fehr, M., Adriaensens, P., Lutsen, L., Vanderzande, D., Maes, W., Goovaerts, E., Van Doorslaer, S. (2014). Electronic structure of positive and negative polarons in functionalized dithienylthiazolo-[5,4-*d*]thiazoles: a combined EPR and DFT study *Physical Chemistry Chemical Physics* 16(21), 10032-10040. <https://doi.org/10.1039/c3cp54635g>

- Behrends, J., Samuel, I.D.W., **Schnegg, A.**, Keeble, D.J. (2013). Persistent spin coherence and bipolarons *Nature Nanotechnology* 8(12), 884-885. <https://doi.org/10.1038/nnano.2013.269>
- Sontheimer, T., Preidel, V., Lockau, D., Back, F., Rudigier-Voigt, E., Lochel, B., Erko, A., Schmidt, F., **Schnegg, A.**, Lips, K., Becker, C., Rech, B. (2013). Correlation between structural and optoelectronic characteristics of crystalline Si microhole arrays for photonic light management *Journal of Applied Physics* 114(17), 173513. <https://doi.org/10.1063/1.4829008>
- Sontheimer, T., **Schnegg, A.**, Steffens, S., Ruske, F., Amkreutz, D., Lips, K., Rech, B. (2013). Identification of intra-grain and grain boundary defects in polycrystalline Si thin films by electron paramagnetic resonance *Physica Status Solidi - Rapid Research Letters* 7(11), 959-962. <https://doi.org/10.1002/pssr.201308061>
- Dikarov, E., Fehr, M., **Schnegg, A.**, Lips, K., Blank, A. (2013). Selective electron spin resonance measurements of micrometer-scale thin samples on a substrate *Measurement Science and Technology* 24(11), 115009. <https://doi.org/10.1088/0957-0233/24/11/115009>
- Nehr Korn, J., Martins, B.M., Holldack, K., Stoll, S., Dobbek, H., Bittl, R., **Schnegg, A.** (2013). Zero-field splittings in metHb and metMb with aquo and fluoro ligands: a FD-FT THz-EPR study *Molecular Physics* 111(18-19), 2696-2707. <https://doi.org/10.1080/00268976.2013.809806>
- Mitchell, D.G., Tseitlin, M., Quine, R.W., Meyer, V., Newton, M.E., **Schnegg, A.**, George, B., Eaton, S.S., Eaton, G.R. (2013). X-band rapid-scan EPR of samples with long electron spin relaxation times: a comparison of continuous wave, pulse and rapid-scan EPR *Molecular Physics* 111(18-19), 2664- 2673. <https://doi.org/10.1080/00268976.2013.792959>
- Meier, C., Behrends, J., Teutloff, C., Astakhov, O., **Schnegg, A.**, Lips, K., Bittl, R. (2013). Multi-frequency EDMR applied to microcrystalline thin-film silicon solar cells *Journal of Magnetic Resonance* 234, 1-9. <https://doi.org/10.1016/j.jmr.2013.06.002>
- Singh, A., Hocking, R.K., Chang, S.L.Y., George, B.M., Fehr, M., Lips, K., **Schnegg, A.**, Spiccia, L. (2013). Water Oxidation Catalysis by Nanoparticulate Manganese Oxide Thin Films: Probing the Effect of the Manganese Precursors *Chemistry of Materials* 25(7), 1098-1108. <https://doi.org/10.1021/cm3041345>
- George, B.M., Behrends, J., **Schnegg, A.**, Schulze, T.F., Fehr, M., Korte, L., Rech, B., Lips, K., Rohrmüller, M., Rauls, E., Schmidt, W.G., Gerstmann, U. (2013). Atomic Structure of Interface States in Silicon Heterojunction Solar Cells *Physical Review Letters* 110(13), 136803. <https://doi.org/10.1103/PhysRevLett.110.136803>
- Dreiser, J., Pedersen, K.S., **Schnegg, A.**, Holldack, K., Nehr Korn, J., Sigrist, M., Tregenna-Piggott, P., Mutka, H., Weihe, H., Mironov, V.S., Bendix, J., Waldmann, O. (2013). Three-Axis Anisotropic Exchange Coupling in the Single-Molecule Magnets  $\text{NEt}_4[\text{Mn}^{\text{III}}_2(5\text{-Brsalen})_2(\text{MeOH})_2\text{M}^{\text{III}}(\text{CN})_6]$  (M=Ru, Os) *Chemistry – A European Journal* 19(11), 3693-3701. <https://doi.org/10.1002/chem.201203781>
- Forshaw, A.P., Smith, J.M., Ozarowski, A., Krzystek, J., Smirnov, D., Zvyagin, S.A., Harris, T.D., Karunadasa, H.I., Zadrozny, J.M., **Schnegg, A.**, Holldack, K., Jackson, T.A., Alamiri, A., Barnes, D.M., Telsler, J. (2013). Low-Spin Hexacoordinate Mn(III): Synthesis and Spectroscopic Investigation of Homoleptic Tris(pyrazolyl)borate and Tris(carbene)borate Complexes *Inorganic Chemistry* 52(1), 144-159. <https://doi.org/10.1021/ic301630d>

## 2012

- Fehr, M., Simon, P., Sontheimer, T., Leendertz, C., Gorka, B., **Schnegg, A.**, Rech, B., Lips, K. (2012). Influence of deep defects on device performance of thin-film polycrystalline silicon solar cells *Applied Physics Letters* 101(12), 123904. <https://doi.org/10.1063/1.4754609>
- Fehr, M., **Schnegg, A.**, Rech, B., Lips, K., Astakhov, O., Finger, F., Freysoldt, C., Bittl, R., Teutloff, C. (2012). Dangling bonds in amorphous silicon investigated by multifrequency EPR *Journal of Non-Crystalline Solids* 358(17), 2067-2070. <https://doi.org/10.1016/j.jnoncrysol.2011.12.105>
- Hoehne, F., Dreher, L., Behrends, J., Fehr, M., Huebl, H., Lips, K., **Schnegg, A.**, Suckert, M., Stutzmann, M., Brandt, M.S. (2012). Lock-in detection for pulsed electrically detected magnetic resonance *Review of Scientific Instruments* 83(4), 43907. <https://doi.org/10.1063/1.4704837>
- Behrends, J., Sperlich, A., **Schnegg, A.**, Biskup, T., Teutloff, C., Lips, K., Dyakonov, V., Bittl, R. (2012). Direct detection of photoinduced charge transfer complexes in polymer fullerene blends *Physical Review B* 85(12), 125206. <https://doi.org/10.1103/PhysRevB.85.125206>
- Salzmann, I., Heimel, G., Duhm, S., Oehzelt, M., Pingel, P., George, B.M., **Schnegg, A.**, Lips, K., Blum, R.P., Vollmer, A., Koch, N. (2012). Intermolecular Hybridization Governs Molecular Electrical Doping *Journal of Physical Chemistry Letters* 108(3), 35502. <https://doi.org/10.1103/PhysRevLett.108.035502>
- **Schnegg, A.**, Behrends, J., Fehr, M., Lips, K. (2012). Pulsed electrically detected magnetic resonance for thin film silicon and organic solar cells *Physical Chemistry Chemical Physics* 14(42), 14418-14438. <https://doi.org/10.1039/c2cp41258f>

## 2011

- Fehr, M., **Schnegg, A.**, Rech, B., Lips, K., Astakhov, O., Finger, F., Pfanner, G., Freysoldt, C., Neugebauer, J., Bittl, R., Teutloff, C. (2011). Combined multifrequency EPR and DFT study of dangling bonds in  $\alpha$ -Si:H *Journal of Physical Chemistry Letters* 84(24), 245203. <https://doi.org/10.1103/PhysRevB.84.245203>
- Fehr, M., Behrends, J., Haas, S., Rech, B., Lips, K., **Schnegg, A.** (2011). Electrical detection of electron-spin-echo envelope modulations in thin-film silicon solar cells *Physical Review B* 84(19), 193202. <https://doi.org/10.1103/PhysRevB.84.193202>
- Dreiser, J., **Schnegg, A.**, Holldack, K., Pedersen, K.S., Schau-Magnussen, M., Nehr Korn, J., Tregenna-Piggott, P., Mutka, H., Weihe, H., Bendix, J., Waldmann, O. (2011). Frequency-Domain Fourier-Transform Terahertz Spectroscopy of the Single-Molecule Magnet  $\text{NEt}_4[\text{Mn}_2(5\text{-Brsalen})_2(\text{MeOH})_2\text{Cr}(\text{CN})_6]$  *Journal of Physical Chemistry Letters* 17(27), 7492-7498. <https://doi.org/10.1002/chem.201100581>
- Muhrer, G., Hartl, M., Daemen, L., Tovesson, F., **Schnegg, A.**, Russina, M., Schachinger, E. (2011). Scattering law of a magnesium hydride moderator *Nuclear Instruments & Methods in Physics Research Section A - Accelerators Spectrometers Detectors and Associated Equipment* 629(1), 251-259. <https://doi.org/10.1016/j.nima.2010.10.144>
- Pedersen, K.S., Dreiser, J., Nehr Korn, J., Gysler, M., Schau-Magnussen, M., Schnegg, A., Holldack, K., Bittl, R., Piligkos, S., Weihe, H., Tregenna-Piggott, P., Waldmann, O., Bendix, J. (2011). A linear single-molecule magnet based on  $[\text{Ru}^{\text{III}}(\text{CN})_6]^{3-}$  *Chemical Communications* 47(24), 6918-6920. <https://doi.org/10.1039/c1cc12158h>

## 2010

- Behrends, J., **Schnegg, A.**, Lips, K., Thomsen, E.A., Pandey, A.K., Samuel, I.D.W., Keeble, D.J. (2010). Bipolaron Formation in Organic Solar Cells Observed by Pulsed Electrically Detected Magnetic Resonance *Physical Review Letters* 105(17), 176601. <https://doi.org/10.1103/PhysRevLett.105.176601>
- Pieper, O., Guidi, T., Carretta, S., van Slageren, J., El Hallak, F., Lake, B., Santini, P., Amoretti, G., Mutka, H., Koza, M., Russina, M., Schnegg, A., Milios, C.J., Brechin, E.K., Julià, A., Tejada, J. (2010). Inelastic neutron scattering and frequency-domain magnetic resonance studies of S=4 and S=12 Mn<sub>6</sub> single-molecule magnets *Physical Review B* 81(17), 174420. <https://doi.org/10.1103/PhysRevB.81.174420>
- Fehr, M., **Schnegg, A.**, Teutloff, C., Bittl, R., Astakhov, O., Finger, F., Rech, B., Lips, K. (2010). Hydrogen distribution in the vicinity of dangling bonds in hydrogenated amorphous silicon (a-Si:H) *Physica Status Solidi A – Applications and Materials Science* 207(3), 552-555. <https://doi.org/10.1002/pssa.200982876>
- Bordignon, E., Brutlach, H., Urban, L., Hideg, K., Savitsky, A., **Schnegg, A.**, Gast, P., Engelhard, M., Groenen, E.J.J., Möbius, K., Steinhoff, H.-J. (2010). Heterogeneity in the Nitroxide Micro-Environment: Polarity and Proticity Effects in Spin-Labeled Proteins Studied by Multi-Frequency EPR *Applied Magnetic Resonance* 37, 391-403. <https://doi.org/10.1007/s00723-009-0072-9>

## 2009

- Behrends, J., **Schnegg, A.**, Fehr, M., Lambertz, A., Haas, S., Finger, F., Rech, B., Lips, K. (2009). Electrical detection of electron spin resonance in microcrystalline silicon pin solar cells *Philosophical Magazine* 89 (28-30), 2655-2676. <https://doi.org/10.1080/14786430903008472>
- Bagryanskaya, E.G., Polovyanenko, DN., Fedin, M.V., Kulik, L., **Schnegg, A.**, Savitsky, A., Mobius, K., Coleman, A.W., Ananchenko, G.S., Ripmeester, J.A. (2009). Multifrequency EPR study of the mobility of nitroxides in solid-state calixarene nanocapsules *Physical Chemistry Chemical Physics* 11(31), 6700-6707. <https://doi.org/10.1039/b906827a>
- **Schnegg, A.**, Behrends, J., Lips, K., Bittl, R., Holldack, K. (2009). Frequency domain Fourier transform THz-EPR on single molecule magnets using coherent synchrotron radiation *Physical Chemistry Chemical Physics* 11(31), 6820-6825. <https://doi.org/10.1039/b905745e>

## 2008

- Behrends, J., **Schnegg, A.**, Boehme, C., Haas, S., Stiebig, H., Finger, F., Rech, B., Lips, K. (2008). Recombination and transport in microcrystalline pin solar cells studied with pulsed electrically detected magnetic resonance *Journal of Non-Crystalline Solids* 354(19-25), 2411-2415. <https://doi.org/10.1016/j.inoncrysol.2007.09.086>
- Okafuji, A., **Schnegg, A.**, Schleicher, E., Möbius, K., Weber, S. (2008). G-tensors of the flavin adenine dinucleotide radicals in glucose oxidase: A comparative multifrequency electron paramagnetic resonance and electron-nuclear double resonance study *Journal of Physical Chemistry B* 112(11), 3568-3574. <https://doi.org/10.1021/jp077170j>

- Polovyanenko, D.N., Bagryanskaya, E.G., **Schnegg, A.**, Möbius, K., Coleman, A.W., Ananchenko, G.S., Udachin, K.A., Ripmeester, J.A. (2008). Inclusion of 4-methoxy-2,2,6,6-tetramethylpiperidine-*N*-oxyl in a calixarene nanocapsule in the solid state *Physical Chemistry Chemical Physics* 10(34), 5299-5307. <https://doi.org/10.1039/b803296c>

## 2007

- **Schnegg, A.**, Dubinskii, A.A., Fuchs, M.R., Grishin, Y.A., Kirilina, E.P., Lubitz, W., Plato, M., Savitsky, A., Möbius, K. (2007). High-field EPR, ENDOR and ELDOR on bacterial photosynthetic reaction centers *Applied Magnetic Resonance* 31(1-2), 59-98. <https://doi.org/10.1007/BF03166248>

## 2006

- **Schnegg, A.**, Kay, C.W.M., Schleicher, E., Hitomi, K., Todo, T., Möbius, K., Weber, S. (2006). The *g*-tensor of the flavin cofactor in (6-4) photolyase: a 360 GHz/12.8 T electron paramagnetic resonance study *Molecular Physics* 104(10-11), 1627-1633. <https://doi.org/10.1080/00268970600593108>
- **Schnegg, A.**, Okafuji, A., Bacher, A., Bittl, R., Fischer, M., Fuchs, M.R., Hegemann, P., Joshi, M., Kay, C.W.M., Richter, G., Schleicher, E., Weber, S. (2006). Towards an identification of chemically different flavin radicals by means of their *g*-tensor *Applied Magnetic Resonance* 30 (3-4), 345-358. <https://doi.org/10.1007/BF03166205>

## 2005

- Kirilina, E.P., Prisner, T.F., Bennati, M., Endeward, B., Dzuba, S.A., Fuchs, M.R., Möbius, K., **Schnegg, A.** (2005). Molecular dynamics of nitroxides in glasses as studied by multi-frequency EPR *Magnetic Resonance in Chemistry* 43(S1), S119-S129. <https://doi.org/10.1002/mrc.1677>
- Möbius, K., Savitsky, A., Wegener, C., Rato, M., Fuchs, M., **Schnegg, A.**, Dubinskii, A.A., Grishin, Y.A., Grigor'ev, I.A., Kühn, M., Duché, D., Zimmermann, H., Steinhoff, H.J. (2005). Combining high-field EPR with site-directed spin labeling reveals unique information on proteins in action *Magnetic Resonance in Chemistry* 43(S1), S4-S19. <https://doi.org/10.1002/mrc.1690>
- Möbius, K., **Schnegg, A.**, Plato, M., Fuchs, M.R., Savitsky, A. (2005). High-field EPR spectroscopy on transfer proteins in biological action *Acta Physica Polonica A* 108(2), 215-234. <https://doi.org/10.12693/APhysPolA.108.215>
- Möbius, K., Savitsky, A., **Schnegg, A.**, Plato, M., Fuchs, M. (2005). High-field EPR spectroscopy applied to biological systems: characterization of molecular switches for electron and ion transfer *Physical Chemistry Chemical Physics* 7(1), 19-42. <https://doi.org/10.1039/b412180e>

## 2004

- Grishin, Y.A., Fuchs, M.R., **Schnegg, A.**, Dubinskii, A.A., Dumesh, B.S., Rusin, F.S., Bratman, V.L., Möbius, K. (2004). Pulsed Orotron - A new microwave source for submillimeter pulse high-field electron paramagnetic resonance spectroscopy *Review of Scientific Instruments* 75(9), 2926-2936. <https://doi.org/10.1063/1.1778071>



## 2003

- Fuchs, M.R., **Schnegg, A.**, Plato, M., Schulz, C., Müh, F., Lubitz, W., Möbius, K. (2003). 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* 294(3), 371-384. [https://doi.org/10.1016/S0301-0104\(03\)00319-7](https://doi.org/10.1016/S0301-0104(03)00319-7)
- Carmieli, R., Manikandan, P., Epel, B., Kalb, A.J., **Schnegg, A.**, Savitsky, A., Möbius, K., Goldfarb, D. (2003). Dynamics in the  $Mn^{2+}$  binding site in single crystals of concanavalin a revealed by high-field EPR spectroscopy *Biochemistry* 42(25), 7863-7870. <https://doi.org/10.1021/bi034281+>

## 2002

- Fuhs, M., **Schnegg, A.**, Prisner, T., Kohne, I., Hanley, J., Rutherford, AW., Möbius, K. (2002). 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 -Bioenergetics* 1556(1), 81-88. [https://doi.org/10.1016/S0005-2728\(02\)00338-9](https://doi.org/10.1016/S0005-2728(02)00338-9)
- **Schnegg, A.**, Fuhs, M., Rohrer, M., Lubitz, W., Prisner, T.F., Möbius, K. (2002). Molecular dynamics of  $Q_A^{-}$  and  $Q_B^{-}$  in photosynthetic bacterial reaction centers studied by pulsed high-field EPR at 95 GHz *Journal of Physical Chemistry B* 106(36), 9454-9462. <https://doi.org/10.1021/jp0203907>
- Fuchs, M.R., Schleicher, E., **Schnegg, A.**, Kay, C.W.M., Törring, J.T., Bittl, R., Bacher, A., Richter, G., Möbius, K., Weber, S. (2002). *g*-tensor of the neutral flavin radical cofactor of DNA photolyase revealed by 360-GHz electron paramagnetic resonance spectroscopy *Journal of Physical Chemistry B* 106(34), 8885-8890. <https://doi.org/10.1021/jp0259869>