## Publikationsliste (peer-reviewed journals and book contributions)

1. S. Lebernegg, G. Amthauer, M Grodzicki. Single-centre MO theory of transition metal complexes. *J. Phys. B* **41** (2008) 035102.

2. S. Lebernegg, G. Amthauer, M. Grodzicki. The d-Hamiltonian - A new approach for evaluating optical spectra of transition metal complexes. *J. Mol. Structure* **924-926** (2009) 473-476.

3. M. Grodzicki, S. Lebernegg. Computation and interpretation of Mössbauer parameters of Fe-bearing compounds. In Book: Mössbauer spectroscopy and transition metal chemistry: Fundamentals and applications. Springer, Berlin 2010.

4. S. Lebernegg, G. Amthauer, M. Grodzicki. Magneto-structural correlations in double-bridged $[Cu_2F_6]^{2-}$. *J. Phys.: Conf. Series* **200** (2010) 032039.

5. S. Lebernegg, G. Amthauer, M. Grodzicki. An analytical approach for calculating transfer integrals in superexchange coupled dimers. *Croat. Chem. Acta* **84** (2011) 39-52.

6. S. Lebernegg. Magneto-structural correlations in doubly hydroxo-bridged Cu(II)-dimers. *Croat. Chem. Acta* **84** (2011) 505-513.

7. S. Lebernegg, A. A. Tsirlin, O. Janson, R. Nath, J. Sichelschmidt, Yu. Skourski, G. Amthauer, H. Rosner; Magnetic model for $A_2CuP_2O_7$ ($A$=Na,Li): One-dimensional versus two-dimensional behavior. *Phys. Rev. B* **84** (2011) 174436.

8. D. Zherebetskyy, S. Lebernegg, G. Amthauer, M. Grodzicki. Magnetic structure of almandine. *Phys. Chem. Minerals* **39** (2012) 351-361.

9. S. Lebernegg, A. A. Tsirlin, O. Janson, H. Rosner. Two energy scales of spin dimers in clinoclase $Cu_3(AsO_4)(OH)_3$. *Phys. Rev. B* **87** (2013) 235117.

10. S. Lebernegg, M. Schmitt, A. A. Tsirlin, O. Janson, H. Rosner. Magnetism of $CuX_2$ frustrated chains ($X$ = F, Cl, Br): Role of covalency. Phys. Rev. B **87** (2013) 155111.

11. A. Tsirlin, O. Janson, S. Lebernegg, Helge Rosner. Square-lattice magnetism of diaboleite $Pb_2Cu(OH)_4Cl_2$. *Phys. Rev. B* **87** (2013) 064404.

12. S. Lebernegg, A. A. Tsirlin, O. Janson, H. Rosner. Spin gap in malachite $Cu_2(OH)_2CO_3$ and its evolution under pressure. *Phys. Rev. B* **88** (2013) 224406.

13. S. Lebernegg, A. A. Tsirlin, O. Janson, H. Rosner. Nearly compensated exchange in the dimer compound callaghanite $Cu_2Mg_2(CO_3)(OH)_6{\cdot}2H_2O$. *Phys. Rev. B* **89** (2014) 165127.

14. S. Lebernegg, A. A. Tsirlin, O. Janson, G. J. Redhammer, H. Rosner. Frustrated magnetic planes with intricate interaction pathways in the mineral langite $Cu_4(OH)_6SO_4 \cdot 2H_2O$. *New J. Phys.* **18** (2016) 033020.

15. S. Lebernegg, O. Janson, S. Nishimoto, I. Rousochatzakis, H. Rosner, A. A. Tsirlin. Frustrated spin chain physics near the Majumdar-Ghosh point in Szenicsite $Cu_3(MoO_4)(OH)_4$. *Phys. Rev. B* **95** (2017) 035145.

16. G. J. Redhammer, A. Senyshyn, S. Lebernegg, G. Tippelt, E. Dachs, G. Roth. A neutron diffraction study of crystal and low-temperature magnetic structures within the $(Na,Li)FeGe_2O_6$ pyroxene-type solid solution series. *Phys. Chem. Minerals* (2017). DOI 10.1007/s00269-017-0892-3.

17. S. Lebernegg, J. Schnack, O. Janson, J. Richter, J. Sichelschmidt, T. Förster, A. A. Tsirlin, H. Rosner. Quantum magnetism in Boleite. *In preparation*.