

## Reviewed publications

Our graduate students are underlined and the journal impact factor (at the time of publication) is given in [brackets].

1. *Analysis of State-Dependent Fluorescence Effects in Multivalent Manganese Oxides and Determination of Electronic Structure*  
P.M. Braun, R.J. Green, A. Moewes, Phys. Rev. Materials 7, 084603 (2023). [4.0]
2. *Determination of Electronic Structure in novel High-Pressure and High-Temperature Phases of Mn<sub>2</sub>O<sub>3</sub>: Exploring Perovskite and Ilmenite Structures*  
P.M. Braun, R.J. Green, S.V. Ovsyannikov, L. Dubrovinsky, A. Moewes, accepted for J. Mat. Chem. C 11, 10864-10871 (2023). [8.1]
3. *Thermally stable red-emitting oxide ceramics for laser lighting*  
Z. Yang, T. de Boer, P.M. Braun, B. Su, Q. Zhang, A. Moewes, Z. Xia, Advanced Materials 35, 2301837 (2023). [32.1]
4. *The Importance of Lone Pairs to Structure and Bonding of the novel Nitridophosphate GeP<sub>2</sub>N<sub>4</sub>*  
T. de Boer, C. Somers, T.D. Boyko, S.J. Ambach, L. Eisenburger, W. Schnick, A. Moewes, J. Mat. Chem. A 11, 6198-6204 (2023). [14.5]
5. *Structural influence of Lone Pairs: GeP<sub>2</sub>N<sub>4</sub>, Representing Germanium(II) Nitridophosphates*  
S.J. Ambach, C. Somers, T. de Boer, L. Eisenburger, A. Moewes, W. Schnick, Angewandte Chemie (Int. Ed.) 135, e202215393 (1 to 5) (2023). [16.8]
6. *Band Gap and Electronic Structure of CaSiN<sub>2</sub> – Experiment and Theory*  
T. de Boer, T.D. Boyko, C. Braun, W. Schnick, A. Moewes, J. Applied Ceramic Technology 20, 197-203 (2023). [2.3]
7. *Structure and Band Gap Determination of InN grown by RP-MOCVD*  
R. Dubreuil, M.R. Amin, J. Tot, M. Nagorski, B. Kadikoff, A. Moewes, D. Alexandrov, J. Materials Science: Materials in Electronics 22, 17668-17677 (2022). [2.8]
8. *Energy Levels of Eu<sup>2+</sup> States in the Next-Generation LED-Phosphor SrLi<sub>2</sub>Al<sub>2</sub>O<sub>2</sub>N<sub>2</sub>:Eu<sup>2+</sup>*  
M.R. Amin, P. Strobel, W. Schnick, P.J. Schmidt, A. Moewes, J. Mat. Chem. C 10, 9740-9747 (2022). [8.1]
9. *Experimental and theoretical characterization of x-ray induced excitons, magnons and dd transitions in MoO<sub>3</sub> nanosheets*  
A. Qamar, P.M. Braun, S. Walia, S. Balendhran, F. Rahman, E.Z. Kurmaev, A. Moewes, Phys. Rev. Materials 6, 074003 (2022). [4.0]
10. *Band Gap and Electronic Structure of Defects in the Ternary Nitride BP<sub>3</sub>N<sub>6</sub>: Experiment and Theory*  
T. de Boer, Md.F. Al Fattah, M.R. Amin, S. Ambach, S. Vogel, W. Schnick, A. Moewes, J. Mat. Chem. C 10, 6429-6434 (2022). [8.1]
11. *Inverse-tunable Red Luminescence and Electronic Properties of Nitridoberyllaluminates Sr<sub>2-x</sub>Ba<sub>x</sub>[BeAl<sub>3</sub>N<sub>5</sub>]:Eu<sup>2+</sup> (x=0–2)*  
E. Elzer, P. Strobel, V. Weiler, M.R. Amin, P.J. Schmidt, A. Moewes, W. Schnick, Chem. – Europ. J. 28, e202104121 (1 to 8) (2022) [5.0]
12. *Detecting a Hierarchy of Deep level defects in the model semiconductor ZnSiN<sub>2</sub>*  
T. de Boer, J. Häusler, P. Strobel, T.D. Boyko, S.S. Rudel, W. Schnick, A. Moewes, J. Phys. Chem. C 1125, 27959-27965 (2021). [4.1]

13. *Tuning the Electronic Bandgap of Oxygen Bearing Cubic Zirconium Nitride:  $c\text{-Zr}_{3-x}(\text{N}_{1-x}\text{O}_x)_4$*   
T.D. Boyko, A. Zerr and A. Moewes, ACS Appl. Electr. Mat. 3, 4768-4773 (2021). [new journal]
14. *Comprehensive Band Gap and Electronic Structure Investigations of the Prominent Phosphors  $\text{M}_2\text{Si}_5\text{N}_8$  ( $\text{M}=\text{Ca}, \text{Sr}, \text{Ba}$ ) Determined Using Soft X-ray Spectroscopy and Density Functional Theory*  
T.M. Tolhurst, C. Braun, W. Schnick, A. Moewes, J. Phys. Chem. C 125, 25799-25806 (2021). [4.1]
15. *Unraveling the Energy Levels of  $\text{Eu}^{2+}$  ions in  $\text{MBe}_{20}\text{N}_{14}:\text{Eu}^{2+}$  ( $\text{M}=\text{Sr}, \text{Ba}$ ) Phosphors*  
M.R. Amin, E. Elzer, W. Schnick, and A. Moewes, J. Phys. Chem. C 125, 11828-11837 (2021). [4.1]
16. *Electronic Properties of Carbyne Chains: Experiment and theory*  
T. de Boer, D. Zatsepin, D. Raikov, E.Z. Kurmaev, A.F. Zatsepin, A. Moewes, J. Phys. Chem. C 125, 8268-8273 (2021). [4.1]
17. *Understanding of luminescence properties using direct measurements on  $\text{Eu}^{2+}$ -doped wide band gap phosphors*  
M.R. Amin, P. Strobel, A. Qamar, T. Giftthaler, W. Schnick, and A. Moewes, Adv. Opt. Mat. 8, 2000504 (2020). [8.3]
18. *Electronic Structure of Wide Band Gap Semiconductors  $\text{Mg}_2\text{PN}_3$  and  $\text{Zn}_2\text{PN}_3$*   
Md.F. Al Fattah, M.R. Amin, M. Mallmann S. Kasap, W. Schnick, and A. Moewes J. Phys.: Cond. Matter 32, 405504 (2020). [2.7]
19. *Origin and control of room temperature ferromagnetism in  $\text{Co}, \text{Zn}$ -doped  $\text{SnO}_2$ : oxygen vacancies and their local environment*  
J. Ho, T. de Boer, B. Leedahl, D. Manikandan, R. Murugan, and A. Moewes, J. Mat. Chem. C 8, 4902-4908 (2020). [6.6]
20. *Direct Evidence of Charge Transfer upon Anion Intercalation in Graphite Cathodes through New Electronic Graphite States: An Experimental and Theoretical Study of Hexafluorophosphate*  
T. de Boer, J. Lapping, J. Read, T. Fister, M. Balasubramanian, J. Cabana, and A. Moewes, Chemistry of Materials 32, 2036-2042 (2020). [10.2]
21. *A probe of Valence and Conduction Band Electronic Structure of Lead Oxide Films for Photodetectors*  
A. Qamar, M. Amin, O. Grynko, O. Semeniuk, A. Reznik, and A. Moewes, ChemPhysChem 20, 3328-3335 (2019). [3.1]
22. *Energy band gaps and excited states in  $\text{Si-QD}/\text{SiO}_x\text{R}_y\text{O}_z$  ( $\text{R}=\text{Si}, \text{Al}, \text{Zr}$ ) suboxide superlattices*  
A.F. Zatsepin, E.A. Buntov, D.A. Zatsepin, E.Z. Kurmaev, V.A. Pustovarov, A.V. Ershov, N.W. Johnson, and A. Moewes, J. Phys.: Cond. Mat. 31, 415301-1-9 (2019). [2.7]
23. *Electronic Structure and Structural Defects in 3d-Metal doped  $\text{In}_2\text{O}_3$*   
J. Ho, J. Becker, B. Leedahl, D.W. Boukhvalov, I.S. Zhidkov, A.I. Khukharenko, E.Z. Kurmaev, S.O. Cholakh, N.V. Gavrilov, V.I. Brinzari, and A. Moewes, J. Mat. Sci.: Mat. in Electronics 30, 14091-14098 (2019). [2.2]
24. *Paving the way towards green catalytic materials for green fuels: impact of chemical species on Mo-based catalysts for hydrodeoxygenation*

- D. Valencia, L. Díaz-García<sup>1</sup>, L.F. Ramírez-Verduzco, A. Qamar, A. Moewes, and J. Aburto, RSC Advances 9, 18292-18301 (2019). [3.0]
25. *Fundamental Crystal Field Excitations in magnetic semiconductor SnO<sub>2</sub>:Mn,Fe,Co,Ni*  
B. Leedahl, D. McClosky, D.W. Boukhvalov, I.S. Zhidkov, A.I. Khukharenko, E.Z. Kurmaev, S.O. Cholakh, N.V. Gavrilov, V.I. Brinzari, and A. Moewes, Phys. Chem. Chem. Phys. 21, 11992-11998 (2019). [3.6]
26. *Bandgap and Electronic Structure Determination of Oxygen-Containing Ammonothermal InN: Experiment and Theory*  
M.R. Amin, T. de Boer, P. Becker, J. Hertrampf, R. Niewa, and A. Moewes, J. Phys. Chem. C 123, 8943-8950 (2019). [4.3]
27. *Oxygen Vacancy Induced Structural Distortions in Black Titania: A unique Approach using Soft X-ray EXAFS at the O-K Edge*  
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28. *Ultrasmall Au nanocatalysts supported on nitride carbon for electrocatalytic CO<sub>2</sub> reduction: the role of the carbon support in high selectivity*  
L. Jin, B. Liu, P. Wang, H. Yao, L.A. Achola, P. Kerns, A. Lopes, Y. Yang, J. Ho, A. Moewes, Y. Pei, and J. He, Nanoscale 10, 14678-14686 (2018). [7.0]
29. *Luminescence of an Oxonitridoberyllate: A Study of Narrow-band Cyan Emitting Sr[Be<sub>6</sub>ON<sub>4</sub>]:Eu<sup>2+</sup>*  
P. Strobel, T. de Boer, V. Weiler, P.J. Schmidt, A. Moewes, and W. Schnick, Chemistry of Materials 30, 3122-3130 (2018). [10.2]
30. *The Electronic structure of ε'-V<sub>2</sub>O<sub>5</sub>: an expanded band gap in a double-layered polymorph with increased interlayer separation*  
T.M. Tolhurst, B. Leedahl, J.L. Andrews, S. Banerjee, A. Moewes, J. Mat. Chem. A 5, 23694-23703 (2017). [10.7]
31. *X-ray spectroscopic study of various lead oxides for direct conversion imaging*  
A. Qamar, K. LeBlanc, J. Lin, Y. Pan, A. Reznik, A. Moewes, Scientific reports 7, 13159 1-10 (2017). [4.0]
32. *Direct measurements of Energy Levels and Correlation with Thermal Quenching behavior in Nitrides Phospors*  
T.M. Tolhurst, P. Strobel, P.J. Schmidt, W. Schnick, A. Moewes, Chem. Mat. 29, 7976-7983 (2017). [10.2]
33. *How functional groups change the electronic structure of graphdiyne: Theory and Experiment*  
N. Ketabi, T.M. Tolhurst, B. Leedahl, H. Liu, Y. Li, A. Moewes, Carbon 123, 1-7 (2017). [7.5]
34. *Recent Advances with Soft X-ray Absorption Spectroscopy*  
A. Moewes, Handbook of Solid State Chemistry, 1<sup>st</sup> edition, 2017, Chapter 11 (pages 361-391) Wiley.
35. *Bulk vs. Surface Structure of 3d Metal impurities in Topological Insulator Bi<sub>2</sub>Te<sub>3</sub>*  
B. Leedahl, D.W. Boukhvalov, E.Z. Kurmaev, A. Kukharenko, I.S. Zhidkov, N.V. Gavrilov, S.O. Cholakh, P. Huu Le, C. Wei Luo, and A. Moewes, Scientific Reports 7, 5758 (2017). [5.2]
36. *Tunability of room-temperature ferromagnetism in Spintronic semiconductors through nonmagnetic atoms*

- B. Leedahl, Z. Talizadeh, K. LeBlanc, A. Moewes, Phys. Rev. B 96, 045202-1-5 (2017). [3.7]
37. *Designing Luminescence Materials and Band Gaps: A Soft X-ray spectroscopy and Density Functional Theory Study of  $\text{Li}_2\text{Ca}_2[\text{Mg}_2\text{Si}_2\text{N}_6]:\text{Eu}^{2+}$  and  $\text{Ba}[\text{Li}_2(\text{Al}_2\text{Si}_2)\text{N}_6]:\text{Eu}^{2+}$*   
T.M. Tolhurst, P. Strobel, W. Schnick, A. Moewes, J. Phys. Chem. C 121, 14296-14301 (2017). [4.5]
38. *Structure-Induced Switching of the Band Gap, Charge Order and Correlation Strength in Ternary Vanadium Bronzes*  
T.M. Tolhurst, J.L. Andrews, B. Leedahl, P.M. Marley, S. Banerjee, and A. Moewes, Chemistry – A European Journal 23, 9846-9856 (2017). [5.8]
39. *Intercalation-induced dimensional reduction and thickness-modulated electronic structure of a layered ternary vanadium oxide*  
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40. *The hardness of group 14 spinel nitrides revisited*  
T.D. Boyko and A. Moewes, Journal of the Ceramic Society of Japan 124, 1063-1066 (2016). [0.83]
41. *Searching for pure iron in nature: magnetic and spectroscopy study of the Chelyabinsk meteorite*  
B. Leedahl, A.V. Korolev, I.S. Zhidkov, S.L. Skornyakov, V.I. Anisimov, A.S. Belozеров, A.I. Kukhareno, E.Z. Kurmaev, V.I. Grokhovskii, S.O. Cholakh, and A. Moewes, RSC Advances 6, 85844-85851 (2016). [3.3]
42. *Experiment-driven modeling of crystalline phosphorus nitride: wide ranging implications from a unique structure*  
T.M. Tolhurst, C. Braun, T.D. Boyko, W. Schnick, A. Moewes, Chemistry – A European Journal 22, 10475-10483 (2016). [5.8]
43. *Tuning the electronic structure of graphene through nitrogen doping: Experiment and theory*  
N. Ketabi, T. de Boer, M. Karakay, J. Zhu, A. Podila, A.M. Rao, E.Z. Kurmaev, and A. Moewes, RSC Advances 6, 56721-56727 (2016). [3.3]
44. *Contrasting 1D Tunnel Structured and 2D Layered Polymorphs of  $\text{V}_2\text{O}_5$ : Relating Structure and Bonding to Band Gaps and Electronic Structure*  
T.M. Tolhurst, B. Leedahl, J.L. Andrews, P.M. Marley, S. Banerjee, and A. Moewes, Phys. Chem. Chem. Phys. 18, 15798-15806 (2016). [4.5]
45. *Band Gap and electronic structure of cubic, rhombohedral, and orthorhombic  $\text{In}_2\text{O}_3$  polymorphs: Experiment and theory*  
T. de Boer, M.F. Bekheet, A. Gurlo, R. Riedel, and A. Moewes, Phys. Rev. B 93, 155205 (2016). [3.7]
46. *Electronic structure, Band gap and thermal quenching of  $\text{Sr}[\text{Mg}_3\text{SiN}_4]:\text{Eu}^{2+}$  and  $\text{Sr}[\text{LiAl}_3\text{N}_4]:\text{Eu}^{2+}$*   
T.M. Tolhurst, S. Schmiechen, P. Pust, P.J. Schmidt, W. Schnick, and A. Moewes, Adv. Opt. Mat. 4, 584-591 (2016). [7.2]

47. *Transition from Reconstruction toward Thin Film on the (110) Surface of Strontium Titanate*  
Z. Wang, A. Loon, A. Subramanian, S. Gerhold, E. McDermott, J.A. Enterkin, M. Hieckel, B.C. Russell, R.J. Green, A. Moewes, J. Guo, P. Blaha, M.R. Castell, U. Diebold, and L.D. Marks, *Nano Letters* 16, 2407-2412 (2016). [13.8]
48. *Oxidized Monolayers of Epitaxial Silicene on Ag(111)*  
N.W. Johnson, D. Muir and A. Moewes, *Scientific Reports* 6, 22510 (2016). [5.6]
49. *Linking the HOMO-LUMO Gap to Torsional Disorder in P3HT/PCBM Blends*  
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50. *Selective Area Band Engineering of Graphene using Cobalt-Mediated Oxidation*  
P. Bazylewski, V.L. Nguyen, R.P.J. Bauer, A.H. Hunt, E.J.G. McDermott, B.D. Leedahl, A.I. Kukharenko, S.O. Cholakh, E.Z. Kurmaev, P. Blaha, A. Moewes, Y.H. Lee, G.S. Chang, *Sci. Reports* 5, 15380 (2015). [5.6]
51. *Adjacent Fe-Vacancy Interactions as the Origin of Room Temperature Ferromagnetism in  $(\text{In}_{1-x}\text{Fe}_x)_2\text{O}_3$*   
R.J. Green, T.Z. Regier, B. Leedahl, J.A. McLeod, X.H. Xu, G.S. Chang, E.Z. Kurmaev, and A. Moewes, *Phys. Rev. Lett.* 115, 167401 (2015). [7.7]
52. *The characterization of Co-nanoparticles supported on graphene*  
P. Bazylewski, D. Boukhvalov, A.I. Kukharenko, E.Z. Kurmaev, A. Hunt, A. Moewes, Y.H. Lee, S.O. Cholakh, and G.S. Chang, *RSC Advances* 5, 75600-75606 (2015). [3.8]
53. *Pronounced, reversible, and in situ modification of the electronic structure of graphene oxide via cooling below 160 K*  
A. Hunt, E. McDermott, E.Z. Kurmaev and A. Moewes, *J. Phys. Chem. Letters* 6, 3163-3169 (2015). [7.5]
54. *Stability and Electronic Characteristics of Epitaxial Silicene Multilayers on Ag(111)*  
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T. de Boer, T.D. Boyko, C. Braun, W. Schnick, and A. Moewes, *physica status solidi – Rapid Research Letters* 9 (4), 250-254 (2015). [2.4]
56. *Investigations of the Electronic Structure and Bandgap of the Next-generation LED-phosphor  $\text{Sr}[\text{LiAl}_3\text{N}_4]:\text{Eu}^{2+}$  – Experiments and calculations*  
T.M. Tolhurst, T.D. Boyko, P. Pust, N.W. Johnson, W. Schnick, and A. Moewes, *Advanced Optical Materials* 3, 546-550 (2015). [7.2]
57. *Electronic structure of  $\text{Li}_2\text{RuO}_3$  studied by LDA+DMFT calculations and X-ray spectroscopy*  
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58. *Determination of the Critical Current Density in  $\text{YBa}_2\text{Cu}_3\text{O}_{7-\delta}$  Thin Films Measured by the Screening Technique Under Two Criteria*  
F. Gamboa, I. Perez, J.A. Matutes-Aquino, A. Moewes, and V. Sosa, *IEEE Transactions on Applied Superconductivity* 25 (1), 8000105 (2015). [1.2]
59. *Study of the Structural Characteristics of 3d metals Cr, Mn, Fe, Co, Ni, and Cu Implanted in ZnO and  $\text{TiO}_2$  – Experiment and Theory*

- B. Leedahl, D.Z. Zatsepin, D.W. Boukhvalov, E.Z. Kurmaev, R.J. Green, I.S. Zhidkov, S.S. Kim, N.V. Gavrilov, S.O. Cholakh, and A. Moewes, *J. Phys. Chem. C* 118, 28143-28151 (2014). [4.8]
60. *Electronic structure and spin trapping in LiMnAs and LiFeAs:Mn*  
J.A. McLeod, E.Z. Kurmaev, I. Perez, R.J. Green, L.Y. Xing, X.C. Wang, C.-Q. Jin, and A. Moewes, *J. Phys. Cond. Matt.* 27, 015504 (2015). [2.2]
61. *Asymmetric pathways in the electrochemical conversion reaction of NiO as battery electrode with high storage capacity*  
U. Boesenberg, M.A. Marcus, A.K. Shukla, T. Yi, E. McDermott, P.F. Teh, M. Srinivasan, A. Moewes, J. Cabana, *Scientific Reports* 4, 7133-7142 (2014). [5.1]
62. *The electronic structure of Zirconium in hydrided and oxidized states*  
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63. *Electronic Structure of FeSe<sub>1-x</sub>Te<sub>x</sub> Studied by X-ray Spectroscopy and Density Functional Theory*  
I. Pérez, J.A. McLeod, R.J. Green, R. Escamilla, V. Ortiz, and A. Moewes, *J. Phys. Chem. C* 118, 25150-25157 (2014). [4.8]
64. *Electronic structure of Co-substituted FeSe superconductor probed by soft X-ray spectroscopy and density functional theory*  
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65. *The Metallic Nature of Epitaxial Silicene Monolayers on Ag(111)*  
N.W. Johnson, P. Vogt, A. Resta, P. De Padova, I. Perez, D. Muir, E.Z. Kurmaev, G. Le Lay, and A. Moewes, *Adv. Func. Mat.* 24, 5253-5259 (2014). [10.4]
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A. Hunt, E.Z. Kurmaev, and A. Moewes, *Advanced Materials* 26, 4870-4874 (2014). [15.4]
67. *Measuring Partial Fluorescence Yield using Filtered Detectors*  
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68. *Band gap engineering of graphene oxide by chemical modification*  
A. Hunt, E.Z. Kurmaev, and A. Moewes, *Carbon* 75, 366-371 (2014). [6.2]
69. *Comment on "State-Dependent Electron Delocalization Dynamics at the Solute-Solvent Interface: Soft X-ray Absorption Spectroscopy and Ab Initio Calculations"*  
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70. *Local Structure of Fe Impurity Atoms in ZnO: Bulk versus Surface*  
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71. *Electronic Band gap reduction and intense luminescence in Co and Mn ion-implanted SiO<sub>2</sub>*  
R.J. Green, D.A. Zatssepin, D.J. St. Onge, E.Z. Kurmaev, N.V. Gavrilov, and A. Moewes, *J. Appl. Phys.* 115, 103708-1-7 (2014). [2.2]
72. *Structural defects induced by Fe-ion implantation in TiO<sub>2</sub>*

- B. Leedahl, D.A. Zatsepin, D.W. Boukhvalov, R.J. Green, J.A. McLeod, S.S. Kim, E.Z. Kurmaev, I.S. Zhidkov, N.V. Gavrilov, S.O. Cholakh, and A. Moewes, *J. Appl. Physics* 115, 053711-1-7 (2014). [2.2]
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77. *Magnesium Double Nitride  $Mg_3GaN_3$  and Binary Nitride  $Mg_3N_2$  as New Host Lattices for  $Eu^{2+}$ -Doping – Synthesis, Structural Studies, Luminescence and Band Gap Determination*  
F. Hintze, N.W. Johnson, M. Seibald, D. Muir, A. Moewes, and W. Schnick, *Chem. Mat.* 25, 4044-4052 (2013). [8.5]
78. *X-ray Spectroscopic Study of the Conduction Band of  $K_3$ :Anthracene and  $K_3$ :Phenanthrene*  
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