

## List of publications

Dr. Gregor Kieslich, Liebig Fellow and TU Munich Junior Fellow

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Number of peer reviewed publications: 64

Number of citations: 3660, h-index: 28 (google scholar, December 2021)

### SCIENTIFIC PUBLICATIONS - OVERVIEW

64. A. L. Semrau, S. V. Dummert, C. Eckel, S. Mackewicz, R. T. Weitz, G. Kieslich\*. Synthetic Approaches Targeting Metal-Free Perovskite [HMDABCO](NH<sub>4</sub>)<sub>3</sub> Thin Films. *Cryst. Growth. Des.* **2022**, 1, 406.
63. P. Vervoorts, J. Stebani, A. S. J. Méndez, G. Kieslich\*. Structural Chemistry of Metal-Organic Frameworks under Hydrostatic Pressures. *ACS Materials Lett.* **2021**, 3, 1635.
62. S. Burger, S. Grover, K. T. Butler, H. L. B. Boström, R. Grau-Crespo\*, G. Kieslich\*. Tilt and Shift Polymorphism in Molecular Perovskites. *Mater. Horiz.* **2021**, 8, 2444.
61. L. Petters, S. Burger, S. Kronawitter, M. Drees, G. Kieslich\*. Linear Negative Thermal Expansion in Pd(acac)<sub>2</sub>. *CrystEngComm.* **2021**, 23, 5425.
60. D. Ukaj, H. Bunzen, J. Berger, G. Kieslich, R. A. Fischer\*. Charge-Transfer-Induced Electrical Conductivity in a Tetrathiafulvalene-Based Metal-Organic Framework. *Chem. Mater.* **2021**, 33, 2532.
59. C. L. Hobday\*, G. Kieslich\*. Structural Flexibility in Crystalline Coordination Polymers: A Journey Along the Underlying Free Energy Landscape. *Dalton. Trans.* **2021**, 50, 3759.
58. C. Kaußler, G. Kieslich\*. crystalT: complexity and configurational entropy of crystal structures via information theory. *J. Appl. Cryst.* **2021**, 54, 306.
57. H. L. B. Boström\*, G. Kieslich\*. Influence of Metal Defects on the Mechanical Properties of ABX<sub>3</sub> Perovskite-Type Metal-formate Frameworks. *J. Phys. Chem. C.* **2021**, 125, 1467.
56. P. Vervoorts, J. Keupp, A. Schneemann, C. L. Hobday, D. Daisenberger, R. A. Fischer, R. Schmid\*, G. Kieslich\*. Configurational Entropy Driven High-Pressure Behaviour of a Flexible Metal-Organic Framework. *Angew. Chem.* **2020**, 60, 787.
55. S. Burger, S. Kronawitter, H. L. B. Boström, J. K. Zareba, G. Kieslich\*. A new polar perovskite coordination network with azaspiroundecane as A-site cation. *Dalton. Trans.* **2020**, 49, 10750.
54. D. Bodesheim, G. Kieslich, M. Johnson, K. T. Butler\*. Understanding the Balance of Entropy and Enthalpy in Hydrogen-Halide Noncovalent Bonding. *J. Phys. Chem. Lett.* **2020**, 11, 3495.
53. C. Schneider, D. Bodesheim, J. Keupp, R. Schmid, G. Kieslich\*. Retrofitting metal-organic frameworks. *Nat. Commun.* **2019**, 10, 4921.
52. Keith T. Butler\*, P. Vervoorts, M. G. Ehrenreich, J. Armstrong, J. M. Skelton, G. Kieslich\*. Experimental Evidence for Vibrational Entropy as Driving Parameter of Flexibility in the Metal-Organic Framework ZIF-4(Zn). *Chem. Mater.* **2019**, 31, 8366-8372.
51. P. Vervoorts, C. L. Hobday, M. G. Ehrenreich, D. Daisenberger, G. Kieslich\*. The Zeolitic Imidazolate Framework ZIF-4 under Low Hydrostatic Pressures. *Z. Anorg. Allg. Chem.* **2019**, 645, 970-974.
50. C. Schneider, D. Bodesheim, M. G. Ehrenreich, V. Crocellà, J. Mink, R. A. Fischer, K. T. Butler, G. Kieslich\*. Tuning the Negative Thermal Expansion Behavior of the Metal-Organic Framework Cu<sub>3</sub>BTC<sub>2</sub> by Retrofitting. *J. Am. Chem. Soc.* **2019**, 141, 10504-10509.
49. D. C. Mayer, A. Manzi, R. Medishetty, B. Winkler, C. Schneider, G. Kieslich, A. Pöthig, J. Feldmann, R. A. Fischer\*. Controlling Multi-Photon Absorption Efficiency by Chromophore Packing in Metal-Organic Frameworks. *J. Am. Chem. Soc.* **2019**, 141, 11594-11602.

48. A. Schneemann, R. Rudolf, S. J. Baxter, P. Vervoorts, I. Hante, K. Khaletskaia, S. Henke, G. Kieslich\*, R. A. Fischer\*. Flexibility control in alkyl ether-functionalized pillared-layered MOFs by a Cu/Zn mixed metal approach. *Dalton Trans.* **2019**, 48, 6564-6570.
47. W. Li, S. Watzel, H. El-sayed, Y. Liang, G. Kieslich, A. S. Bandarenka, K. Rodewald, B. Rieger, R. A. Fischer\*. Unprecedented High Oxygen Evolution Activity of Electrocatalysts Derived from Surface-Mounted Metal-Organic Frameworks. *J. Am. Chem. Soc.* **2019**, 141, 5926-5933.
46. C. Ott, F. Reiter, M. Baumgartner, M. Pielmeier, A. Vogel, P. Walke, S. Burger, M. G. Ehrenreich, G. Kieslich\*, D. Daisenberger, J. Armstrong, U. K. Thakur, P. Kumar, S. Chen. D. Donadio, L. S. Walter, R. T. Weitz, K. Shankar\*, T. Nilges\*. Flexible and Ultrasoft 1D Semiconductor and Heterostructure Systems Based on SnIP. *Adv. Funct. Mater.* **2019**, 29, 1900233.
45. M. G. Ehrenreich, Z. Zeng, S. Burger, M. R. Warren, M. W. Gaultois, J.-C. Tan\*, G. Kieslich\*. Mechanical Properties of the ferroelectric metal-free perovskites [MDABCO](NH<sub>4</sub>)I<sub>3</sub>. *Chem. Commun.* **2019**, 55, 3911-3914.
44. A. Regoutz, A. M. Ganose, L. Blumenthal, C. Schlueter, T.-L. Lee, G. Kieslich, A. K. Cheetham, G. Kerherve, Y.-S. Huang, R.-S. Chen, G. Vinai, T. Pincelli, G. Panaccione, K. H. L. Zhang, R. G. Egdell, J. Lischner, D. O. Scanlon, D. J. Payne\*. Insights into the electronic structure of OsO<sub>2</sub> using soft and hard X-ray photoelectron spectroscopy in combination with density functional theory. *Phys. Rev. Materials* **2019**, 3, 025001.
43. S. Wannapaiboon, A. Schneemann, I. Hante, M. Tu, K. Epp, A. L. Semrau, C. Sternemann, M. Paulus, S. Baxter, G. Kieslich, R. A. Fischer\*. Control of structural flexibility of layered-pillared metal-organic frameworks anchored at surfaces. *Nat. Commun.* **2019**, 10, 346.
42. G. Kieslich\*, J. M. Skelton, J. Armstrong, Y. Wu, F. Wei, K. L. Svane, A. Walsh, K. T. Butler\*. Hydrogen Bonding versus Entropy: Revealing the Underlying Thermodynamics of the Hybrid Organic-Inorganic Perovskites [CH<sub>3</sub>NH<sub>3</sub>]<sub>3</sub>PbBr<sub>3</sub>. *Chem. Mater.* **2018**, 30, 8782-8788.
41. S. Leukel, M. Panthöfer, M. Mondeshki, G. Kieslich, Y. Wu, N. Krautwurst, W. Tremel\*. Trapping Amorphous Intermediates of Carbonates – A combined Total Scattering and NMR Study. *J. Am. Chem. Soc.* **2018**, 140, 14638-14646.
40. Z. Deng, G. Kieslich, P.D. Bristowe, A. K. Cheetham\*, S. Sun. Octahedral connectivity and its role in determining the phase stabilities and electronic structures of low-dimensional, perovskite-related iodoplumbates. *APL Materials*, **2018**, 6, 114202.
39. S. Burger, M. Ehrenreich, G. Kieslich\*. Tolerance Factors of hybrid perovskites: recent improvements and current state of research. *J. Mater. Chem. A* **2018**, 6, 21785-21793.
38. S. Dissegna, P. Vervoorts, C. L. Hobday, T. Düren, D. Daisenberger, A. J. Smith, R. A. Fischer\*, G. Kieslich\*. Tuning the Mechanical Response of Metal-Organic Frameworks by Defect-Engineering. *J. Am. Chem. Soc.* **2018**, 140, 11581-11584.
37. S. Leukel, M. Panthöfer, M. Mondeshki, G. Kieslich, Y. Wu, N. Krautwurst, W. Tremel\*. Mechanochemical Access to Defect-Stabilized Amorphous Calcium Carbonate. *Chem. Mater.* **2018**, 30, 6040-6052.
36. C. Schneider, D. Ukaj, R. Koerver, A. A. Talin, G. Kieslich, S. P. Pujari, H. Zuilhof, J. Janek, M. D. Allendorf\*, R. A. Fischer\*. High electrical conductivity and high porosity in a Guest@MOF material: evidence of TCNQ ordering within Cu<sub>3</sub>BTC<sub>2</sub> micropores. *Chem. Sci.* **2018**, 9, 7405-7412.

35. C. Dietrich, R. Koerver, M. W. Gaultois, G. Kieslich, G. Cibir, J. Janek\*, W. G. Zeier\*. Spectroscopic characterization of lithium thiophosphates by XPS and XAS – a model to help monitor interfacial reactions in all-solid-state batteries. *Phys. Chem. Chem. Phys.* **2018**, 20, 20088-20095.
34. G. Cerreti, B. Balke, G. Kieslich, W. Tremel\*. Towards higher zT in early transition metal oxides: optimizing the charge carrier concentration in the WO<sub>3-x</sub> compounds. *Mater. Today: Proceedings* **2018**, 5, 10240-10248.
33. A. K. Cheetham, G. Kieslich\*, H.-M. H. Yeung\*. Thermodynamic and Kinetic Effects in the Crystallization of Metal-Organic Frameworks. *Acc. Chem. Res.* **2018**, 51, 659-667.
32. S. Dissegna, K. Epp, W. R. Heinz, G. Kieslich\*, R. A. Fischer\*. Defective Metal-Organic Frameworks. *Adv. Mater.* **2018**, 30, 1704501.
31. S. Henke, M. T. Wharmby, G. Kieslich, I. Hante, A. Schneemann, Y. Wu, D. Daisenberger, A. K. Cheetham\*. Pore closure in the zeolitic imidazolate frameworks under mechanical pressure. *Chem. Sci.* **2018**, 9, 1654-1660.
30. K. L. Svane, A. C. Forse, C. P. Grey, G. Kieslich, A. K. Cheetham, A. Walsh, K. T. Butler\*. How Strong is the Hydrogen Bond in Hybrid Perovskites? *Phys. Chem. Lett.* **2017**, 8, 6154-6159.
29. S. Dissegna, R. Hardian, K. Epp, G. Kieslich, M.-V. Coulet, P. Llewellyn, R. A. Fischer\*. Using water adsorption measurements to access the chemistry of defects in the metal-organic framework UiO-66. *Cryst. Eng. Comm.* **2017**, 19, 4137-4141.
28. G. Kieslich\*, A. Goodwin. The same and note the same: Molecular perovskites and their solid-state analogues. *Mater. Horiz.* **2017**, 4, 362-366.
27. S. Sun, Z. Deng, Y. Wu, F. Wei, F. H. Isikgor, F. Brivio, M. W. Gaultois, J. Ouyang, P.D. Bristowe, A. K. Cheetham\*, G. Kieslich\*. Variable temperature and high-pressure crystal chemistry of perovskite formamidinium lead iodide: A single crystal X-ray diffraction and computational study. *Chem. Commun.* **2017**, 53, 7537-7540.
26. S. Sun, F. H. Isikgor, Z. Deng, F. Wei, G. Kieslich, P. D. Bristowe, J. Ouyang, A. K. Cheetham\*. Factors Influencing the Mechanical Properties of Formamidinium Lead Halide and Related Hybrid Perovskites. *Chem. Sus. Chem.* **2017**, 10, 3740-3745.
25. F. Wei, Z. Deng, S. Sun, F. Zhang, D. M. Evans, G. Kieslich, S. Tominaka, M. A. Carpenter, J. Zhang, P. D. Bristowe, A. K. Cheetham\*. Synthesis and Properties of a Lead-Free Hybrid Double Perovskite: (CH<sub>3</sub>NH<sub>3</sub>)<sub>2</sub>AgBiBr<sub>6</sub>. *Chem. Mater.* **2017**, 29, 1089-1094.
24. W. Zhang, M. Kauer, P. Guo, S. Kunze, S. Cwik, M. Muhler, Y. Wang, K. Epp, G. Kieslich, R. A. Fischer\*. Impact of Synthesis Parameters on the Formation of Defects in HKUST-1. *Eur. J. Inorg. Chem.* **2017**, 5, 925-932.
23. K. T. Butler\*, K. Svane, G. Kieslich\*, A. K. Cheetham, A. Walsh. Microscopic origin of entropy driven polymorphism in hybrid organic-inorganic perovskite materials. *Phys. Rev. B* **2016**, 94, 180103.
22. K. T. Butler\*, A. Walsh, A. K. Cheetham, G. Kieslich\*. Organised chaos: entropy in hybrid inorganic-organic systems and other materials. *Chem. Sci.* **2016**, 7, 6316-6324.

21. Z. Deng, F. Wei, S. Sun, G. Kieslich, A. K. Cheetham, P. D. Bristowe\*. Exploring the properties of lead-free hybrid double perovskites using a combined computational-experimental approach. *J. Mater. Chem. A* **2016**, 4, 12025-12029.
20. G. Kieslich, G. Cerretti, I. Veremchuk, R. P. Hermann, M. Panthöfer, Y. Grin, W. Tremel\*. A chemists view: Metal oxides with adaptive structures for thermoelectric applications. *Phys. Status Solidi A* **2016**, 213, 808-823.
19. G. Kieslich\*, A. C. Forse, K. T. Butler, S. Kumagai, Y. Wu, M. R. Warren, A. Walsh, C. P. Grey, A. K. Cheetham\*. Role of Amine-Cavity Interactions in Determining Structure and Mechanical Properties of the Ferroelectric Hybrid Perovskite  $[\text{NH}_3\text{NH}_2]\text{Zn}(\text{HCOO})_3$ . *Chem. Mater.* **2016**, 28, 312-317.
18. G. Kieslich\*, S. Kumagai, A. C. Forse, S. Sun, S. Henke, M. Yamashita, C. P. Grey, A. K. Cheetham\*. Tuneable mechanical and dynamical properties in the ferroelectric perovskite solid solution  $[\text{NH}_3\text{NH}_2]_{1-x}[\text{NH}_3\text{OH}]_x\text{Zn}(\text{HCOO})_3$ . *Chem. Sci.* **2016**, 7, 5108-5112.
17. F. Wei, Z. Deng, S. Sun, F. Xie, G. Kieslich, D. M. Evans, M. A. Carpenter, P. D. Bristowe, A. K. Cheetham\*. The synthesis, structure and electronic properties of a lead-free hybrid inorganic-organic double perovskites  $(\text{MA})_2\text{KBiCl}_6$  (MA = methylammonium). *Mater. Horiz.* **2016**, 3, 328-332.
16. Y. Wu, S. Henke, G. Kieslich, I. Schwedler, M. Yang, D. A. X. Fraser, D. O'Hare\*. Time-Resolved In Situ X-ray Diffraction Reveals Metal-Dependent Metal-Organic Framework Formation. *Angew. Chem.* **2016**, 128, 14287-14290.
15. W. Zhang, K. Freitag, S. Wannapaiboon, C. Schneider, K. Epp, G. Kieslich\*, R. A. Fischer. Elaboration of a Highly Porous  $\text{Ru}^{\text{II,III}}$  Analogue of HKUST-1. *Inorg. Chem.* **2016**, 55, 12492-12495.
14. G. Kieslich\*, S. Kumagai, K. T. Butler, T. Okamura, C. H. Hendon, S. Sun, M. Yamashita, A. Walsh, A. K. Cheetham\*. Role of entropic effects in controlling the polymorphism in formate  $\text{ABX}_3$  metal-organic frameworks. *Chem. Commun.* **2015**, 51, 15538-15541.
13. G. Kieslich\*, S. Sun, A. K. Cheetham\*. An extended Tolerance Factor approach for organic-inorganic perovskites. *Chem. Sci.* **2015**, 6, 3430-3433.
12. S. Sun, Y. Fang, G. Kieslich, T. J. White, A. K. Cheetham\*. Mechanical properties of organic-inorganic halide perovskites,  $\text{CH}_3\text{NH}_3\text{PbX}_3$  (X= I, Br and Cl), by nanointendation. *J. Mater. Chem. A* **2015**, 3, 18450-18455.
11. T. Claudio, D. Bessas, C. S. Birkel, G. Kieslich, M. Panthöfer, I. Sergueev, W. Tremel, R. P. Hermann\*. Enhanced Debye level in nano  $\text{Zn}_{1+x}\text{Sb}$ ,  $\text{FeSb}_2$  and  $\text{NiSb}$ : Nuclear inelastic spectroscopy on  $^{121}\text{Sb}$ . *Phys. Status Solidi B* **2014**, 251, 919-923.
10. G. Kieslich, C. S. Birkel, I. Veremchuk, Y. Grin\*, W. Tremel\*. Thermoelectric properties of spark-plasma sintered nanoparticulate  $\text{FeSb}_2$  prepared via a solution chemistry approach. *Dalton Trans.* **2014**, 43, 558-562.
9. G. Kieslich\*, S. Sun, A. K. Cheetham\*. Solid-state principles applied to organic-inorganic perovskites: New tricks for an old dog. *Chem. Sci.* **2014**, 5, 4712-4715.
8. G. Kieslich, U. Burkhardt, C. S. Birkel, I. Veremchuk, J. E. Douglas, M. W. Gaultois, I. Lieberwirth, R. Seshadri, G. D. Stucky, Y. Grin\*, W. Tremel\*. Enhanced thermoelectric properties of the n-type Magnéli phase  $\text{WO}_{2.90}$ : Reduced thermal conductivity through microstructure engineering. *J. Mater. Chem. A* **2014**, 2, 13492-13497.

7. G. Kieslich\*, W. Tremel\*. Magnéli oxides as promising n-type thermoelectrics. *AIMS Materials Science* **2014**, 1, 184-190.
6. W. G. Zeier, C. P. Heinrich, T. Day, C. Panithipongwut, G. Kieslich, G. Brunklaus, G. J. Snyder, W. Tremel\*. Bond strength dependent superionic phase transformation in the solid solution series  $\text{Cu}_2\text{ZnGeSe}_{4-x}\text{S}_x$ . *J. Mater. Chem. A* **2014**, 2, 1790-1794.
5. G. Kieslich, C. S. Birkel, J. E. Douglas, M. Gaultois, I. Veremchuk, R. Seshadri, G. Stucky, Y. Grin, W. Tremel\*. SPS-assisted preparation of the Magnéli phase  $\text{WO}_{2.90}$  for thermoelectric applications. *J. Mater. Chem. A* **2013**, 13050.
4. G. Kieslich, I. Veremchuk, I. Antonyshyn, W. G. Zeier, C. S. Birkel, K. Weldert, C. P. Heinrich, E. Visnow, M. Panthöfer, U. Burkhardt, Y. Grin\*, W. Tremel\*. Using crystallographic shear to reduce lattice thermal conductivity: High temperature thermoelectric characterization of the spark plasma sintered Magnéli phases  $\text{WO}_{2.90}$  and  $\text{WO}_{2.722}$ . *Phys. Chem. Chem. Phys.* **2013**, 15, 15399-15403.
3. C. S. Birkel, T. Claudio, M. Panthöfer, A. Birkel, D. Koll, G. Kieslich, J. Schmidt, R. P. Hermann\*, W. Tremel\*. Properties of spark plasma sintered nanostructured  $\text{Zn}_{1+x}\text{Sb}$ . *Phys. Status Solidi A* **2011**, 208, 1913-1919.
2. C. S. Birkel, G. Kieslich, D. Bessas, T. Claudio, R. Branscheid, U. Kolb, M. Panthöfer, R. P. Hermann\*, W. Tremel\*. Wet chemical synthesis and a combined X-ray and Mössbauer study of the formation of  $\text{FeSb}_2$  nanoparticles. *Inorg. Chem.* **2011**, 50, 11807-11812.
1. G. Kieslich, C. S. Birkel, A. Stewart, U. Kolb, W. Tremel\*. Solution synthesis of nanoparticulate binary transition metal antimonides. *Inorg. Chem.* **2011**, 50, 6938-6943.