

List of publications

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

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Number of peer reviewed publications: 60

Number of citations: 2916, h-index: 26 (google scholar, March 2021)

SCIENTIFIC PUBLICATIONS - OVERVIEW

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**, just accepted: 10.1021/acs.chemmater.0c04897.
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*. crystIT: 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 ABX₃ 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 azaspirodecane 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 Cu₃BTC₂ 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. Khaletskaya, 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. Watzele, 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](NH₄)₃. *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 OsO₂ 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 [CH₃NH₃]PbBr₃. *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 Cu₃BTC₂ 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. Cerretti, B. Balke, G. Kieslich, W. Tremel*. Towards higher zT in early transition metal oxides: optimizing the charge carrier concentration in the WO_{3-x} 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: (CH₃NH₃)₂AgBiBr₆. *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.
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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 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 Zn_{1+x}Sb , FeSb_2 and NiSb : Nuclear inelastic spectroscopy on ^{121}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 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.
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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.

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