

Publications in scientific journals (peer-reviewed)

2021

[30] A. Mutschke, Th. Wylezich, A. D. Sontakke, M. Hoelzel, A. Meijerink, **N. Kunkel***, $\text{ACaH}_x\text{F}_{3-x}$ ($\text{A}=\text{Rb}, \text{Cs}$): Synthesis, structure and bright, site-sensitive tunable Eu^{2+} luminescence, *Adv. Opt. Mater.* **2021**, 2002052, DOI: doi.org/10.1002/adom.202002052.

[29] A. Mutschke, G. M. Bernard, M. Bertmer, A. J. Karttunen, C. Ritter, V. K. Michaelis, **N. Kunkel***, $\text{Na}_3\text{SO}_4\text{H}$ – the first representative of the material class of sulphate hydrides, *Angew. Chem. Int. Ed.*, accepted, DOI: doi.org/10.1002/ange.202016582.

2020

[28] Th. Wylezich, R. Valois, M. Suta, A. Mutschke, C. Ritter, A. Meijerink, A. J. Karttunen, **N. Kunkel***, Borate hydrides as a new material class – Structure, computational studies and spectroscopic investigations on $\text{Sr}_5(\text{BO}_3)_3\text{H}$ and $\text{Sr}_5(^{11}\text{BO}_3)_3\text{D}$, *Chem. Eur. J.* **2020**, 51, 11742-11750, DOI: 10.1002/chem.202002273 (Hot paper, Cover Feature).

[27] J. Ueda*, T. Wylezich, **N. Kunkel***, S. Tanabe, Design Concept by Covalency and Crystal Field for 5d-4f Red Luminescence: Eu^{2+} in $n=1$ Ruddlesden-Popper-type K_2MgH_4 , *J. Mater. Chem. C.*, **2020**, 8, 5124-5130.

2019

[26] A. Mutschke, Th. Wylezich, C. Ritter, A. Karttunen, **N. Kunkel***, An unprecedented fully H^- -substituted phosphate hydride $\text{Sr}_5(\text{PO}_4)_3\text{H}$ expanding the apatite family, *Eur. J. Inorg. Chem.* **2019**, 48, 5073-5076, DOI: 10.1002/ejic.201901151.

[25] Th. Wylezich, A. D. Sontakke, V. Castaing, M. Suta, B. Viana, A. Meijerink, **N. Kunkel***, One ion, many facets: Efficient, structurally and thermally sensitive luminescence of Eu^{2+} in binary and ternary strontium borohydride chlorides, *Chem. Mater.* **2019**, 31, 8957-8968, DOI: 10.1021/acs.chemmater.9b03048.

[24] Th. Wylezich, R. Böttcher, A. Sontakke, V. Castaing, B. Viana, A. Pöppel, **N. Kunkel***, Lanthanide ions as local probes in ionic hydrides: A pulsed electron nuclear double resonance and persistent luminescence study of Eu^{2+} -doped hydride perovskites, *J. Phys. Chem. C* **2019**, 123, 5031-5041, DOI: 10.1021/acs.jpcc.8b12420.

[23] D. Rudolph, Th. Wylezich, Atul D. Sontakke, A. Meijerink, Ph. Goldner, Ph. Netzsche, H. A. Höppe, **N. Kunkel***, Th. Schleid*, Synthesis and Optical Properties of the Eu^{2+} -doped alkaline-earth metal hydride chlorides $\text{AE}_7\text{H}_{12}\text{Cl}_2$ ($\text{AE} = \text{Ca}, \text{Sr}$), *J. Lumin.* **2019**, 209, 150-155, DOI: 10.1016/j.jlumin.2019.01.03.

[22] **Review: N. Kunkel***, Th. Wylezich, Recent Advances in Rare Earth-Doped Hydrides, *Z. Anorg. Allg. Chem.*, **2019**, 645, 137-145, DOI: 10.1002/zaac.201800408, **cover feature Z. Anorg. Allg. Chem. 3/2019** (Dedicated issue).

2018

[21] Th. Wylezich, S. Welinski, M. Hözel, Ph. Goldner, **N. Kunkel***, Lanthanide luminescence as a local probe in mixed anionic hydrides – A case study on Eu^{2+} -doped $\text{RbMgH}_x\text{F}_{3-x}$ and $\text{KMgH}_x\text{F}_{3-x}$, *J. Mat. Chem. C* **2018**, 6, 13006-13012, DOI: 10.1039/C8TC03881C.

[20] G. Lefevre, S. Saitzek, R. Defeux, **N. Kunkel**, A. Sayede*, Hydrogen storage in MgX ($\text{X} = \text{Ba}, \text{Co}, \text{Cu}, \text{Ni}, \text{Ti}, \text{V}$) systems – is there still news? *J. Power Sources* **2018**, 402, 394-401. DOI:

doi.org/10.1016/j.jpowsour.2018.09.043.

[19] G. Lefevre, A. Herfurth, H. Kohlmann, A. Sayede, Th. Wylezich, S. Welinski, P. Duarte Vaz, S. F. Parker, J. F. Blach, Ph. Goldner, **N. Kunkel***, Phonon-electron coupling in luminescent europium doped hydride perovskites studied by luminescence spectroscopy, inelastic neutron scattering, and first-principle calculations, *J. Phys. Chem. C* **2018**, 122, 10501-10509, DOI: 10.1021/acs.jpcc.8b01011.

[18] **Review: N. Kunkel***, Ph. Goldner*, Recent Advances in Rare Earth Doped Inorganic Crystalline Materials for Quantum Information Processing, *Z. Anorg. Allg. Chem.* **2018**, 644, 66-76, DOI: 10.1002/zaac.201700425, **front cover picture Z. Anorg. Allg. Chem 2/2018**. (Dedicated issue).

2017

[17] J. Karlsson*, **N. Kunkel**, A. Ikesue, A. Ferrier, Ph. Goldner, Nuclear spin coherence properties of $^{151}\text{Eu}^{3+}$ and $^{153}\text{Eu}^{3+}$ in a Y_2O_3 transparent ceramic, *J. Phys.: Condens. Matter* **2017**, 29, 125501 (7pp), DOI: 10.1088/1361-648X/aa529a. (**highlighted in J. Phys.: Condens. Matter News and Views**).

2016

[16] **N. Kunkel***, Atul D. Sontakke, S. Kohaut, B. Viana, P. Dorenbos, Thermally simulated luminescence and first-principle study of defect configurations in the perovskite-type hydrides $\text{LiMH}_3:\text{Eu}^{2+}$ ($\text{M} = \text{Sr}, \text{Ba}$) and the corresponding deuterides, *J. Phys. Chem. C* **2016**, 120, 29414-29422, DOI: 10.1021/acs.jpcc.6b10088.

[15] **N. Kunkel***, J. Bartholomew, S. Welinski, A. Ferrier, A. Ikesue, Ph. Goldner, Dephasing mechanisms of optical transitions in rare earth doped transparent ceramics, *Phys. Rev. B : Condens. Matter Mat. Phys.* **2016**, 94, 184301(1-9), DOI : 10.1103/PhysRevB.94.184301.

[14] **N. Kunkel***, J. Bartholomew, L. Binet, A. Ikesue, Ph. Goldner, High resolution optical linewidth measurements as a materials characterization tool, *J. Phys. Chem. C* **2016**, 120, 13725-13731, DOI: 10.1021/acs.jpcc.6b03337.

[13] W. Li, V. R. Celinski, J. Weber, **N. Kunkel**, H. Kohlmann, J. Schmedt auf der Günne*, Doping homogeneity for doping with paramagnetic ions by NMR, *Phys. Chem. Chem. Phys.* **2016**, 18, 9752-9757, DOI: 10.1039/c5cp07606d.

[12] **N. Kunkel***, H. Kohlmann, Ionic mixed hydride fluoride compounds: stabilities predicted by DFT, synthesis and luminescence of divalent europium, *J. Phys. Chem. C* **2016**, 120, 10506-10511, DOI: 10.1021/acs.jpcc.6b00386.

[11] **N. Kunkel***, R. Böttcher, T. Pilling, H. Kohlmann, A. Pöpli, Eu^{2+} -containing luminescent perovskite-type hydrides studied by electron paramagnetic resonance, *Z. Phys. Chem.* **2016**, 230, 931-942, DOI: 10.1515/zpch-2015-0690.
(Dedicated issue).

2015

[10] **N. Kunkel***, A. Ferrier, C. W. Thiel, M. O. Ramírez, L. E. Bausá, R. L. Cone, A. Ikesue, Ph. Goldner*, Rare-earth doped transparent ceramics for spectral filtering and quantum information processing, *Appl. Phys. Lett. Mat.* **2015**, 3, 096103, DOI: 10.1063/1.4930221.

[9] **N. Kunkel**, D. Rudolph, A. Meijerink, S. Rommel, R. Weihrich, H. Kohlmann*, Th. Schleid*, Green luminescence of divalent europium in the mixed anion compound EuHCl , *Z. Anorg. Allg. Chem.* **2015**, 641, 1220-1224, DOI: 10.1002/zaac.201400531. (**Cover picture**)
(Dedicated issue).

[8] R. Hahn, **N. Kunkel**, C. Hein. R. Kautenburger, H. Kohlmann*, Recovery rate and homogeneity of doping europium into luminescent metal hydrides by chemical analysis, *RSC Adv.* **2015**, 5, 9722-9728 DOI: 10.1039/c4ra14076a.

[7] **N. Kunkel***, C. Reichert, M. Springborg, D. Wallacher, H. Kohlmann*, Hydrogenation properties of $\text{Li}_x\text{Sr}_{1-x}\text{AlSi}$ studied by quantum-chemical methods ($0 \leq x \leq 1$) and in situ neutron powder diffraction ($x = 1$), *J. Solid State Chem.* **2015**, 221, 318-324 DOI: 10.1016/j.jssc.2014.10.021.

2014

[6] **N. Kunkel***, A Meijerink, H. Kohlmann*, Variation of the Eu(II) emission wavelength by substitution of fluoride by hydride in $\text{EuH}_x\text{F}_{2-x}$, *Inorg. Chem.* **2014**, 53, 4800-4802, DOI: 10.1021/ic500744s.

[5] **N. Kunkel***, A. Meijerink, M. Springborg, H. Kohlmann*, Eu(II) luminescence in the perovskite host lattices KMgH_3 , NaMgH_3 and mixed crystals $\text{LiBa}_x\text{Sr}_{1-x}\text{H}_3$, *J. Mat. Chem. C* **2014**, 2, 4799-4804 DOI: 10.1039/c4tc00644e.

[4] **N. Kunkel***, A. Meijerink, H. Kohlmann*, Bright yellow and green Eu(II) luminescence and vibronic fine structures in LiSrH_3 , LiBaH_3 and their corresponding deuterides, *Phys. Chem. Chem. Phys.* **2014**, 16, 4807-4813 DOI: 10.1039/c3cp55102d.

[3] J. N. Becker, J. Bauer, A. Giehr, P. I. Chu, **N. Kunkel**, M. Springborg* and H. Kohlmann, Electronic structure of ternary rhodium hydrides with lithium and magnesium, *Inorg. Chem.* **2014**, 50, 1135-1143, DOI: 10.1021/ic402687p.

2011

[2] **N. Kunkel**, H. Kohlmann*, A. Sayede, M. Springborg, Alkaline-Earth Metal Hydrides as Novel Host Lattices for Eu^{II} Luminescence, *Inorg. Chem.* **2011**, 50, 5873-5875, DOI: 10.1021/ic200801x.

[1] **N. Kunkel**, J. Sander, N. Louis, Y. Pang, L.-M. Dejon, F. Wagener, Y. N. Zang, A. Sayede, M. Bauer, M. Springborg*, H. Kohlmann, Theoretical investigation of the hydrogenation induced atomic rearrangements in palladium rich intermetallic compounds MPd₃ (M = Mg, In, Tl), *Eur. Phys. J. B* **2011**, 82, 1-6, DOI: 10.1140/epjb/e2011-10916-5.

Other publications (non-peer-reviewed)

[6] I. Hartenbach, **N. Kunkel**, C. Benndorf, H. Terraschke, Trendbericht Festkörperchemie, *Nachrichten aus der Chemie* **2020**, 68 (Februar), 34-44, DOI 10.1002/nadc.20204094620.

Blickpunkt Anorganische Chemie/Nachrichten aus der Chemie 2019:

[5] **N. Kunkel***, O. Clemens*, Daten speichern im Kristallgitter, *Nachrichten aus der Chemie* **2019**, 67 (Dezember), 47-50, DOI: 10.1002/nadc.20194090189.

[4] O. Clemens*, **N. Kunkel***, Ordnung in der Ordnung, *Nachrichten aus der Chemie* **2019**, 67 (Oktober), 62-66, DOI: 10.1002/nadc.20194090183.

[3] **N. Kunkel***, O. Clemens*, M. Suta, Sieh mal, Seltene Erden, *Nachrichten aus der Chemie* **2019**, 67 (Juli/August), 71-75, DOI: 10.1002/nadc.20194089019.

[2] **N. Kunkel***, O. Clemens*, M. Hözel, A. Senyshyn, Strukturen, Zusammensetzung, Mechanismen, *Nachrichten aus der Chemie* **2019**, 67 (Juni), 66-69, DOI: 10.1002/nadc.20194085457.

- [1] O. Clemens*, N. Kunkel*, Mit dem richtigen Dreh die Thermodynamik überlisten, *Nachrichten aus der Chemie* **2019**, 67, 59-62, DOI: 10.1002/nadc.20194083930.

Invited talks

2020

[26] N. Kunkel, Novel Luminescence Materials, Plenary Talk, Joint MLZ User Meeting & German Neutron Scattering Conference 2020, 10.12.2020, online.

[25] N. Kunkel, Rare earth ions as local probes and some novel mixed anionic hydrides, Inorganic Chemistry Seminar, Oxford, 03.11.2020, online.

2019

[24] N. Kunkel, Novel Mixed Anionic Hydrides, GDCh-Weihnachtskolloquium, 12.12.2019, Georg-August-Universität Göttingen, Germany.

[23] N. Kunkel, Leuchtendes mit H, Quantenspeicher und mehr..., Bier und Brezel Vortrag, 29.11.2019, Georg-August-Universität Göttingen, Germany.

[22] N. Kunkel, Optische Sonden, neue Materialien und Quantenspeicher, Westfälische Wilhelms-Universität Münster, 22.10.2019, Münster, Germany.

[21] N. Kunkel, Rare earth ions – Local probes and quantum technologies, New Trends in Inorganic Chemistry, Universität des Saarlandes, 12.09.2019, Saarbrücken, Germany.

[20] N. Kunkel, Illuminating hydrides – rare earth metal ions as local probes, Göttinger Chemie-Forum, 04.07.2019, Georg-August-Universität Göttingen, Germany.

[19] N. Kunkel, Seltene Erden – von Lumineszenz, lokalen Sonden und Quantenspeichern, 21.05.2019, Universität Kiel (AC-Kolloquium), Germany.

[18] N. Kunkel, Rare Earth Ions as Local Probes and for Optical Materials, 03.05.2019, Molecules Meet Solids – Inorganic Chemistry with Focus on Novel Materials, TU Munich, Garching, Germany.

[17] N. Kunkel, Materialien für Energie- und optische Anwendungen, Otto-von-Guericke-University Magdeburg, 05.03.2019, Germany.

2018

[16] N. Kunkel, Rare earth ions as local probes for novel materials and quantum information, 17.12.2018, Physics Seminar Series (Seminario Dpto. Física de Materiales), Facultad de Ciencias, Universidad Autónoma de Madrid, Spain.

[15] N. Kunkel, Rare earth ions as local probes for novel materials and quantum information, 09.08.2018, Chemistry and Material Science Seminar Series, Aalto University, Espoo, Finland.

[14] N. Kunkel, Rare earth ions as local probes in hydrides, 25.06.2018, TU Darmstadt, Germany.

[13] N. Kunkel, Seltene Erden – von Lumineszenz, lokalen Sonden und Quantenspeichern, 21.06.2018, Rheinische Friedrich-Wilhelms-Universität Bonn (AC-Kolloquium), Bonn, Germany.

[12] N. Kunkel, Rare-earth ions as local probes in hydrides and mixed anionic hydrides, 21.

Steinheimer Gespräche für den Hochschullehrernachwuchs, 14.-16.06.2018, Mainz, Germany.

[11] N. Kunkel, Materialien für Energie- und optische Anwendungen, Georg-August-Universität Göttingen, 04.05.2018, Germany.

[10] N. Kunkel, Schwingungsspektroskopische Untersuchungen von Substitutionseffekten in Hydriden und Hydrid-Fluoriden sowie deren Deuteriden, 25.01.2018, Ladenburg, Germany.

2017

[9] N. Kunkel, Design and characterization of optical materials with europium, September 2017, Université d'Artois, France.

[8] N. Kunkel, T. Wylezich, Illuminating hydrides, AC@TUM Get Together Symposium, 24.-25.04.2017, TUM Academy Center Raitenhaslach, Germany.

[7] N. Kunkel, Synthese und optische Eigenschaften europiumhaltiger Verbindungen, 08.03.2017, LMU Munich (AC Sonderkolloquium), Germany.

2016

[6] N. Kunkel, From an experimentalist's point of view- How theory can complement the experiment, From Atoms via Molecules to Solids – A Symposium on Theoretical Studies Dedicated to Prof. Michael Springborg on the Occasion of his 60th Birthday, 21.-22.04.2016, Saarbrücken, Germany.

[5] N. Kunkel, Design und Charakterisierung europiumdotierter Materialien für optische Anwendungen, Technische Universität Dortmund, 23.02.2016, Germany.

2015

[4] N. Kunkel, C. Reichert, M. Springborg, D. Wallacher, H. Kohlmann, Hydrogenation properties of $\text{Li}_x\text{Sr}_{1-x}\text{AlSi}$ studied by quantum-chemical methods ($0 \leq x \leq 1$) and in-situ neutron powder diffraction ($x = 1$), 7th Joint BER II and BESSY II User Meeting, 2015, Helmholtz Zentrum Berlin, Germany.

[3] N. Kunkel, Talk at the award ceremony of the Dr. Eduard-Martin foundation, 22.10.2015, Saarbrücken, Germany.

[2] N. Kunkel, Europium – von Lumineszenz und Metallhydriden zu Quantenspeichern, Georg-August-Universität Göttingen, 26. 03. 2015, Germany.

[1] N. Kunkel, Leuchtende Metallhydride mit Eu(II) – Talk at the award ceremony of the Wilhelm-Klemm foundation, Hemdsärmelkolloquium 2015, Munich, Germany.

Conference talks

2020

[17] T. Wylezich, A. Mutschke, N. Kunkel*, Structurally and thermally sensitive luminescence of Eu²⁺ in borohydride chlorides and novel mixed-anionic hydrides, Online-Vortragstagung für Anorganische Chemie der Fachgruppen Wöhler-Vereinigung und Festkörperchemie und Materialforschung 2020.

[16] N. Kunkel, Local probes and novel mixed-anionic hydrides, ERC-IC Webinar Series 2020, 22.07.2020.

2019

- [15] N. Kunkel, Rare earth ions as local probes in novel mixed-anionic hydrides and designing materials using (de)hydrogenation reactions, ATUMS Annual Meeting, 10.-15.11.2019, Canmore, Canada.
- [14] T. Wylezich, A. Mutschke, N. Kunkel, Optical properties of rare earth doped mixed anionic hydrides and borohydrides, Tage der Seltenen Erden – Terraer Rarae 2019, 30.05-01-06.2019, Stockholm, Sweden.
- [13] N. Kunkel, Optical probes and energy materials, SFB1073 Winter School 2019, 10.-14.02.2019, Hirscheegg, Austria.

2018

- [12] N. Kunkel, Rare Earth ions as local probes for materials and for quantum information, 2nd Germany-Brazil Bilateral Workshop ‘New light on mechanisms of chemical reactions’, 04.12.-06.12.2018, São Paulo, Brazil.
- [11] N. Kunkel, Rare earth luminescence in hydrides (Invited session introductory talk), 28.08.2018, 5th International Conference on the Physics of Optical Materials and Devices, Igalo, Montenegro.
- [10] N. Kunkel, Leuchtendes mit H, Hemdsärmelkolloquium 2018, Leipzig, Germany

2016

- [9] N. Kunkel, Ph. Goldner, Coherence spectroscopy as a tool for the characterization of local environments of rare-earth doped materials, Annual meeting of the German Crystallographic Society (DGK) 2016, Stuttgart, Germany.

2015

- [8] N. Kunkel, A. Ferrier, C. W. Thiel, M. O. Ramírez, L. E. Bausá, R. L. Cone, A. Ikesue, Ph. Goldner, Narrow inhomogeneous linewidths and long spectral hole lifetimes in Eu³⁺-doped highly transparent ceramics, 5th IWASOM, 2015, Gdansk, Poland.
- [7] N. Kunkel, Atomare Kohärenz trotz Unordnung?, Hemdsärmelkolloquium 2015, Munich, Germany.

2014

- [6] N. Kunkel, A. Meijerink, H. Kohlmann, Eu(II)-Lumineszenz in hydridischen Perowskiten, Mitteldeutsches Anorganiker Nachwuchssymposium, 2014, Freiberg, Germany.
- [5] N. Kunkel, A. Meijerink, H. Kohlmann, Eu(II) luminescence in mixed hydride fluorides and overview on hydride host lattices, Terraer Rarae, 2014, Köln, Germany.
- [4] N. Kunkel, Eu(II) als Aktivator in hydridischen Perowskitgittern, Seminar zur Festkörperchemie 2014, Hirscheegg, Austria.

2013

- [3] N. Kunkel, A. Meijerink, H. Kohlmann, Bright yellow and green luminescence of Eu(II) in LiMH₃ and LiMD₃ (M=Sr, Ba) and the first observation of a vibronic fine structure in the spectra of Eu(II) in a hydridic matrix, Terraer Rarae, 2013, Stuttgart, Germany.

2012

[2] N. Kunkel, Leuchtende Europiumhydride, Gesamtkolloquium der Graduiertenförderung der Hochschulen des Saarlandes 2012, Saarbrücken, Germany.

2011

[1] N. Kunkel, Lumineszenz von Europium in Erdalkalihydriden, Seminar zur Festkörperchemie, 2011, Hirschegg, Austria.