Curriculum Vitae

Univ.-Prof. Dr. rer. nat.

Karsten Albe

Dipl.-Phys.

Date and place of birth:
03.11.1967, Hildesheim, Germany

Technische Universität Darmstadt
Fachbereich Material- und Geowissenschaften
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October 2020

Curriculum Vitae

Professional Employment Record

08/2007 – present	**Professor (W2)**, Materials Modeling Division, Institute of Materials Science, TU Darmstadt *Modeling of defects in materials for energy conversion and storage, substitution materials and novel nanostructured metals and glasses,* *Particle-based simulation methods and their combination,* *Development of data analysis tools*
10/2008 – 03/2009	**Visiting Professor**, VirginiaTech, Blacksburg, USA
11/2002 – 07/2007	**Junior Professor (W1)**, Materials Modeling Division, Institute of Materials Science, TU Darmstadt
07/2000 – 10/2002	**Research Associate**, Thin Films Division (with Prof. Dr. Horst Hahn), Institute of Materials Science, TU Darmstadt *Nanocrystalline Metals, Gas-Phase Synthesis of Nanoparticles, Van-der-Waals Crystals*
08/1998 – 06/2000	**Postdoctoral Research Associate**, Materials Research Laboratory (Prof. Dr. Robert Averback) and Center for Simulation of Advanced Rockets, University of Illinois, Urbana-Champaign, USA *Interatomic Potentials for Compound Materials, Heterogeneous Interfaces, Ion-Solid Interaction*
10/1994 – 07/1998	**Research Assistant**, Research Center Rossendorf-Dresden, Institute of Ion Beam Physics and Materials Research (with Prof. Dr. Wolfhard Möller) *Structure and Growth of Superhard Coatings*
05/1994 – 09/1994	**Research Assistant**, Department of Experimental Physics (with Prof. Dr. Hans-G. Kilian), University of Ulm

Education

08/2005	Positive Interim-Evaluation of Junior-Professorship (equivalent to Habilitation)
06/07/1998	**Doctorate** (*Dr. rer. nat.*) in Physics, TU Dresden *Doctoral Thesis (summa cum laude): "Computer Simulations on Structure and Growth of Boron Nitride"*
02/05/1994	**Diploma (Dipl.-Phys.)** in Physics, University of Ulm *Diploma Thesis: "Isobaric Phase Diagrams and Structure of Crystallizing Mixtures of Higher 1-Mono-Carboxylic Acids"*
10/1990 – 05/1994	University of Ulm, Study of Physics
10/1988 – 09/1990	University of Hamburg, Study of Physics (Intermediate Diploma)
07/1987 – 09/1988	Compulsory Military Service
05/1987	**University-Entrance Diploma** (Abitur), Gymnasium Andreanum, Hildesheim

Further Academic Activities

04/2020 – present	**Dean**, Department of Materials- and Geosciences, TU Darmstadt
04/2020 – present	Elected **Member of the DFG Review Panel 406 "Materials Science"**
10/2015 – present	**Member of the Advisory Board** of "Hessischer Hochleistungsrechner Lichtenberg"
04/2012 –03/2016	Elected **Member of the DFG-Review Panel "Materials Science"**
04/2012 –12/2014	**Spokesperson of SFB 595**, Collaborative Research Center "Electric Fatigue in Functional Materials''
2010 – 2015	**Member of the Scientific Council** of the John von Neumann-Institute for Computing (NIC)
2010, 2012, 2014	**Topic Organizer** "Modeling" MSE Congress, Darmstadt
04/2005 – 12/2008	**Deputy Editor** of Scripta Materialia

06/2005 – 07/2007 | **Member of the University Assembly** of TU Darmstadt

Awards and Distinctions

05/1997 | *€-MRS–Young Scientist Award*
12/1998 | *Graduate Student Award*, Research Center Rossendorf-Dresden

Professional Society Memberships

Materials Research Society
Deutsche Physikalische Gesellschaft
Deutsche Gesellschaft für Materialkunde
Gesellschaft für Angewandte Mathematik und Mechanik
Deutscher Hochschulverband

Reviewing

Deutsche Forschungsgemeinschaft
Humboldt Foundation
National Science Foundation
European Research Council

Science
Nature, Nature Materials, Nature Communications
Physical Review Letters
Physical Review B
Physical Review Materials
Acta Materialia
Scripta Materialia
Journal of Applied Physics
Applied Physics Letters
Journal of Physics: Cond. Mat.
Material Research Letters
Journal of Alloys & Compounds
Intermetallics
Computational Materials Science
Modeling and Simulation in Materials Science & Engineering
Journal Power Sources
Thin Solid Films
Philosophical Magazine A
Journal of Crystal Growth
Nuclear Instruments and Methods B
Applied Surface Science
Journal of Materials Research

Invited Talks (last 5 years)

ISMANAM, Chennai (2019)
DPG-Frühjahrstagung Regensburg (2019)
APS Meeting Boston (2019)
Sino-German Symposium, Münster (2019)
CECAM-Workhshop, Bremen (2018)
Mechanics of Multifunctional Materials, Bad Honnef (2018)
Controversial Colloquium on Grain Boundaries, Irvine (2018)
FZ Rossendorf-Dresden, Festvortrag (2017)
RQ 16, Leoben (2017)
Batterieworkshop, Gießen (2017)
Int. Workshop on Hysteresis in magnetocaloric, electrocaloric and elastocaloric refrigeration Dresden (2017)
MSE, Darmstadt (2016)
EMCS, Santiago de Compostella (2016)
DPG Frühjahrstagung, Regensburg (2016)
EMA, Orlando (2016)
DPG Frühjahrstagung, Berlin (2015)

Supervised Theses since 2002

11 Diploma Theses
20 Master Theses
18 (+ 11 ongoing) Doctoral Theses

Bibliometric Details

ORCID-ID	0000-0003-4669-8056
ResearcherID	F-1139-2011

Research Profile and Publications (October 2020)

"Our ambition is to explain or predict defect properties by computational methods based on solid-state physics, statistical and materials mechanics."

The research of my team is focused on modeling of defects in materials. Areas of interest are:

- Nanostructured materials and glasses
- Materials for energy conversion and storage
- Functional oxides

Our key competences are:

- Modeling the influence of point defects, dislocations, interfaces and interphases on electronic, structural, mechanical and kinetic material properties
- Modeling of material properties and processes with quantum mechanical methods (density functional theory), atomistic many-body methods (Molecular Dynamics, Monte Carlo) and multiscale methods
- Development of visualization and analysis methods

Nanoglasses

[1] C. Kalcher, O. Adjaoud, and K. Albe, Creep deformation of a Cu-Zr nanoglass and interface reinforced nanoglass-composite studied by molecular dynamics simulations, FRONTIERS IN MATERIALS **7** (2020) 10.3389/fmats.2020.00223.

[2] S. H. Nandam, O. Adjaoud, R. Schwaiger, Y. Ivanisenko, M. R. Chellali, D. Wang, K. Albe, and H. Hahn, Influence of topological structure and chemical segregation on the thermal and mechanical properties of Pd-Si nanoglasses, ACTA MATERIALIA **193**, 252–260 (2020).

[3] O. Adjaoud and K. Albe, Influence of microstructural features on the plastic deformation behavior of metallic nanoglasses, ACTA MATERIALIA **168**, 393–400 (2019).

[4] Y. Ivanisenko, C. Kübel, S. H. Nandam, C. Wang, X. Mu, O. Adjaoud, K. Albe, and H. Hahn, Structure and properties of nanoglasses, ADVANCED ENGINEERING MATERIALS **20** (2018) 10.1002/adem.201800404.

[5] O. Adjaoud and K. Albe, Microstructure formation of metallic nanoglasses: insights from molecular dynamics simulations, ACTA MATERIALIA **145**, 322–330 (2018).

[6] C. Kalcher, O. Adjaoud, J. Rohrer, A. Stukowski, and K. Albe, Reinforcement of nanoglasses by interface strengthening, SCRIPTA MATERIALIA **141**, 115–119 (2017).

[7] O. Adjaoud and K. Albe, Interfaces and interphases in nanoglasses: surface segregation effects and their implications on structural properties, ACTA MATERIALIA **113**, 284–292 (2016).

[8] D. Sopu and K. Albe, Influence of grain size and composition, topology and excess free volume on the deformation behavior of Cu-Zr nanoglasses, BEILSTEIN JOURNAL OF NANOTECHNOLOGY **6**, 537–545 (2015).

[9] Y. Ritter and K. Albe, Chemical and topological order in shear bands of $Cu_{64}Zr_{36}$ and $Cu_{36}Zr_{64}$ glasses, JOURNAL OF APPLIED PHYSICS **111** (2012) 10.1063/1.4717748.

[10] Y. Ritter, D. Sopu, H. Gleiter, and K. Albe, Structure, stability and mechanical properties of internal interfaces in $Cu_{64}Zr_{36}$ nanoglasses studied by MD simulations, ACTA MATERIALIA **59**, 6588–6593 (2011).

[11] Y. Ritter and K. Albe, Thermal annealing of shear bands in deformed metallic glasses: recovery mechanisms in $Cu_{64}Zr_{36}$ studied by molecular dynamics simulations, ACTA MATERIALIA **59**, 7082–7094 (2011).

[12] D. Sopu, J. Kotakoski, and K. Albe, Finite-size effects in the phonon density of states of nanostructured germanium: a comparative study of nanoparticles, nanocrystals, nanoglasses, and bulk phases, PHYSICAL REVIEW B **83** (2011) 10.1103/PhysRevB.83.245416.

[13] D. Sopu, Y. Ritter, H. Gleiter, and K. Albe, Deformation behavior of bulk and nanostructured metallic glasses studied via molecular dynamics simulations, PHYSICAL REVIEW B **83** (2011) 10.1103/PhysRevB.83.100202.

[14] D. Sopu, K. Albe, Y. Ritter, and H. Gleiter, From nanoglasses to bulk massive glasses, APPLIED PHYSICS LETTERS **94** (2009) 10.1063/1.3130209.

Metallic Glasses and Composites

[15] C. Kalcher, T. Brink, J. Rohrer, A. Stukowski, and K. Albe, Elastostatic loading of metallic glass-crystal nanocomposites: relationship of creep rate and interface energy, PHYSICAL REVIEW MATERIALS **3** (2019) 10.1103/PhysRevMaterials.3.093605.

[16] D. Sopu, K. Albe, and J. Eckert, Metallic glass nanolaminates with shape memory alloys, ACTA MATERIALIA **159**, 344–351 (2018).

[17] T. Brink and K. Albe, From metallic glasses to nanocrystals: molecular dynamics simulations on the crossover from glass-like to grain-boundary-mediated deformation behaviour, ACTA MATERIALIA **156**, 205–214 (2018).

[18] C. Kalcher, T. Brink, J. Rohrer, A. Stukowski, and K. Albe, Interface-controlled creep in metallic glass composites, ACTA MATERIALIA **141**, 251–260 (2017).

[19] T. Brink, M. Peterlechner, H. Roesner, K. Albe, and G. Wilde, Influence of crystalline nanoprecipitates on shear-band propagation in Cu-Zr-based metallic glasses, PHYSICAL REVIEW APPLIED **5** (2016) 10.1103/PhysRevApplied.5.054005.

[20] T. Brink, D. Sopu, and K. Albe, Solid-state amorphization of Cu nanolayers embedded in a $Cu_{64}Zr_{36}$ glass, PHYSICAL REVIEW B **91** (2015) 10.1103/PhysRevB.91.184103.

[21] K. A. Avchaciov, Y. Ritter, F. Djurabekova, K. Nordlund, and K. Albe, Effect of ion irradiation on structural properties of $Cu_{64}Zr_{36}$ metallic glass, NUCLEAR INSTRUMENTS & METHODS IN PHYSICS RESEARCH SECTION B-BEAM INTERACTIONS WITH MATERIALS AND ATOMS **341**, 22–26 (2014).

[22] J. Bünz, T. Brink, K. Tsuchiya, F. Meng, G. Wilde, and K. Albe, Low temperature heat capacity of a severely deformed metallic glass, PHYSICAL REVIEW LETTERS **112** (2014) 10.1103/PhysRevLett.112.135501.

[23] K. Albe, Y. Ritter, and D. Sopu, Enhancing the plasticity of metallic glasses: shear band formation, nanocomposites and nanoglasses investigated by molecular dynamics simulations, MECHANICS OF MATERIALS **67**, 94–103 (2013).

[24] K. A. Avchaciov, Y. Ritter, F. Djurabekova, K. Nordlund, and K. Albe, Controlled softening of $Cu_{64}Zr_{36}$ metallic glass by ion irradiation, APPLIED PHYSICS LETTERS **102** (2013) 10.1063/1.4804630.

[25] S. Mayr, Y. Ashkenazy, K. Albe, and R. Averback, Mechanisms of radiation-induced viscous flow: role of point defects, PHYSICAL REVIEW LETTERS **90** (2003) 10.1103/PhysRevLett.90.055505.

High Entropy Alloys

[26] J. Kottke, D. Utt, M. Laurent-Brocq, A. Fareed, D. Gärtner, L. Perriere, L. Rogal, A. Stukowski, K. Albe, S. Divinski V, and G. Wilde, Experimental and theoretical study of tracer diffusion in a series of $CoCrFeMn_{(100-x)}Ni_x$ alloys, ACTA MATERIALIA **194**, 236–248 (2020).

[27] F. Thiel, D. Utt, A. Kauffmann, K. Nielsch, K. Albe, M. Heilmaier, and J. Freudenberger, Breakdown of varvenne scaling in $(AuNiPdPt)_{(1-x)}Cu_x$ high-entropy alloys, SCRIPTA MATERIALIA **181**, 15–18 (2020).

[28] D. Utt, A. Stukowski, and K. Albe, Grain boundary structure and mobility in high-entropy alloys: a comparative molecular dynamics study on a Σ 11 symmetrical tilt grain boundary in face-centered cubic CuNiCoFe, ACTA MATERIALIA **186**, 11–19 (2020).

[29] F. Thiel, D. Geissler, K. Nielsch, A. Kauffmann, S. Seils, M. Heilmaier, D. Utt, K. Albe, M. Motylenko, D. Rafaja, and J. Freudenberger, Origins of strength and plasticity in the precious metal based high-entropy alloy AuCuNiPdPt, ACTA MATERIALIA **185**, 400–411 (2020).

[30] E. Levo, F. Granberg, D. Utt, K. Albe, K. Nordlund, and F. Djurabekov, Radiation stability of nanocrystalline single-phase multicomponent alloys, JOURNAL OF MATERIALS RESEARCH **34**, 854–866 (2019).

[31] L. Koch, F. Granberg, T. Brink, D. Utt, K. Albe, F. Djurabekova, and K. Nordlund, Local segregation versus irradiation effects in high-entropy alloys: steady-state conditions in a driven system, JOURNAL OF APPLIED PHYSICS **122** (2017) 10.1063/1.4990950.

[32] T. Brink, L. Koch, and K. Albe, Structural origins of the boson peak in metals: from high-entropy alloys to metallic glasses, PHYSICAL REVIEW B **94** (2016) 10.1103/PhysRevB.94.224203.

Nanoporous Metals

[33] B.-N. D. Ngo, B. Roschning, K. Albe, J. Weissmüller, and J. Markmann, On the origin of the anomalous compliance of dealloying-derived nanoporous gold, SCRIPTA MATERIALIA **130**, 74–77 (2017).

[34] B.-N. D. Ngo, A. Stukowski, N. Mameka, J. Markmann, K. Albe, and J. Weissmüller, Anomalous compliance and early yielding of nanoporous gold, ACTA MATERIALIA **93**, 144–155 (2015).

[35] P. Erhart, E. Bringa, M. Kumar, and K. Albe, Atomistic mechanism of shock-induced void collapse in nanoporous metals, PHYSICAL REVIEW B **72** (2005) 10.1103/PhysRevB.72.052104.

Nanocrystalline Materials

[36] J. Schäfer, A. Stukowski, and K. Albe, On the hierarchy of deformation processes in nanocrystalline alloys: grain boundary mediated plasticity vs. dislocation slip, JOURNAL OF APPLIED PHYSICS **114** (2013) 10.1063/1.4821763.

[37] A. Kobler, J. Lohmiller, J. Schäfer, M. Kerber, A. Castrup, A. Kashiwar, P. A. Gruber, K. Albe, H. Hahn, and C. Kübel, Deformation-induced grain growth and twinning in nanocrystalline palladium thin films, BEILSTEIN JOURNAL OF NANOTECHNOLOGY **4**, 554–566 (2013).

[38] J. Schäfer and K. Albe, Plasticity of nanocrystalline alloys with chemical order: on the strength and ductility of nanocrystalline Ni-Fe, BEILSTEIN JOURNAL OF NANOTECHNOLOGY **4**, 542–553 (2013).

[39] J. Schäfer and K. Albe, Competing deformation mechanisms in nanocrystalline metals and alloys: coupled motion versus grain boundary sliding, ACTA MATERIALIA **60**, 6076–6085 (2012).

[40] J. Schäfer, Y. Ashkenazy, K. Albe, and R. S. Averback, Effect of solute segregation on thermal creep in dilute nanocyrstalline Cu alloys, MATERIALS SCIENCE AND ENGINEERING A-STRUCTURAL MATERIALS PROPERTIES MICROSTRUCTURE AND PROCESSING **546**, 307–313 (2012).

[41] J. Schäfer and K. Albe, Influence of solutes on the competition between mesoscopic grain boundary sliding and coupled grain boundary motion, SCRIPTA MATERIALIA **66**, 315–317 (2012).

[42] N. Q. Vo, J. Schäfer, R. S. Averback, K. Albe, Y. Ashkenazy, and P. Bellon, Reaching theoretical strengths in nanocrystalline Cu by grain boundary doping, SCRIPTA MATERIALIA **65**, 660–663 (2011).

[43] J. Schäfer, A. Stukowski, and K. Albe, Plastic deformation of nanocrystalline Pd-Au alloys: on the interplay of grain boundary solute segregation, fault energies and grain size, ACTA MATERIALIA **59**, 2957–2968 (2011).

[44] A. Stukowski, K. Albe, and D. Farkas, Nanotwinned fcc metals: strengthening versus softening mechanisms, PHYSICAL REVIEW B **82** (2010) 10.1103/PhysRevB.82.224103.

[45] A. Stukowski, J. Markmann, J. Weissmüller, and K. Albe, Atomistic origin of microstrain broadening in diffraction data of nanocrystalline solids, ACTA MATERIALIA **57**, 1648–1654 (2009).

[46] Z.-H. Jin, P. Gumbsch, K. Albe, E. Ma, K. Lu, H. Gleiter, and H. Hahn, Interactions between non-screw lattice dislocations and coherent twin boundaries in face-centered cubic metals, ACTA MATERIALIA **56**, 1126–1135 (2008).

[47] S.-J. Zhao, K. Albe, and H. Hahn, Grain size dependence of the bulk modulus of nanocrystalline nickel, SCRIPTA MATERIALIA **55**, 473–476 (2006).

[48] Z.-H. Jin, P. Gumbsch, E. Ma, K. Albe, K. Lu, H. Hahn, and H. Gleiter, The interaction mechanism of screw dislocations with coherent twin boundaries in different face-centred cubic metals, SCRIPTA MATERIALIA **54**, 1163–1168 (2006).

[49] W. Voegeli, K. Albe, and H. Hahn, Simulation of grain growth in nanocrystalline nickel induced by ion irradiation, NUCLEAR INSTRUMENTS & METHODS IN PHYSICS RESEARCH SECTION B-BEAM INTERACTIONS WITH MATERIALS AND ATOMS **202**, 230–235 (2003).

Nanoparticles

[50] A. Tolvanen and K. Albe, Plasticity of Cu nanoparticles: dislocation-dendrite-induced strain hardening and a limit for displacive plasticity, BEILSTEIN JOURNAL OF NANOTECHNOLOGY **4**, 173–179 (2013).

[51] P. M. Diehm, P. Agoston, and K. Albe, Size-dependent lattice expansion in nanoparticles: reality or anomaly?, CHEMPHYSCHEM **13**, 2443–2454 (2012).

[52] J. Pohl, C. Stahl, and K. Albe, Size-dependent phase diagrams of metallic alloys: a Monte Carlo simulation study on order-disorder transitions in Pt-Rh nanoparticles, BEILSTEIN JOURNAL OF NANOTECHNOLOGY **3**, 1–11 (2012).

[53] D. Gross, R. Müller, M. Müller, B.-X. Xu, and K. Albe, On the origin of inhomogeneous stress and strain distributions in single-crystalline metallic nanoparticles, INTERNATIONAL JOURNAL OF MATERIALS RESEARCH **102**, 743–747 (2011).

[54] M. Müller and K. Albe, Kinetic lattice Monte-Carlo simulations on the ordering kinetics of free and supported FePt $L1_0$-nanoparticles, BEILSTEIN JOURNAL OF NANOTECHNOLOGY **2** (2011) 10.3762/bjnano.2.5.

[55] T. T. Järvi, A. Kuronen, K. Nordlund, and K. Albe, Damage production in nanoparticles under light ion irradiation, PHYSICAL REVIEW B **80** (2009) 10.1103/PhysRevB.80.132101.

[56] T. T. Järvi, A. Kuronen, K. Nordlund, and K. Albe, Low energy cluster deposition of nanoalloys, JOURNAL OF APPLIED PHYSICS **106** (2009) 10.1063/1.3225910.

[57] T. T. Järvi, D. Pohl, K. Albe, B. Rellinghaus, L. Schultz, J. Fassbender, A. Kuronen, and K. Nordlund, From multiply twinned to fcc nanoparticles via irradiation-induced transient amorphization, EPL **85** (2009) 10.1209/0295-5075/85/26001.

[58] T. T. Järvi, A. Kuronen, K. Nordlund, and K. Albe, Structural modification of a multiply twinned nanoparticle by ion irradiation: a molecular dynamics study, JOURNAL OF APPLIED PHYSICS **102** (2007) 10.1063/1.2825045.

[59] M. Müller and K. Albe, Structural stability of multiply twinned FePt nanoparticles, ACTA MATERIALIA **55**, 6617–6626 (2007).

[60] M. Müller, P. Erhart, and K. Albe, Thermodynamics of l1(0) ordering in FePt nanoparticles studied by Monte Carlo simulations based on an analytic bond-order potential, PHYSICAL REVIEW B **76** (2007) 10.1103/PhysRevB.76.155412.

[61] M. Müller and K. Albe, Concentration of thermal vacancies in metallic nanoparticles, ACTA MATERIALIA **55**, 3237–3244 (2007).

[62] T. T. Järvi, A. Kuronen, K. Meinander, K. Nordlund, and K. Albe, Contact epitaxy by deposition of Cu, Ag, Au, Pt, and Ni nanoclusters on (100) surfaces: size limits and mechanisms, PHYSICAL REVIEW B **75** (2007) 10.1103/PhysRevB.75.115422.

[63] P. Krasnochtchekov, K. Albe, Y. Ashkenazy, and R. Averback, Molecular-dynamics study of the density scaling of inert gas condensation, JOURNAL OF CHEMICAL PHYSICS **123** (2005) 10.1063/1.2074247.

[64] P. Erhart and K. Albe, Molecular dynamics simulations of gas phase condensation of silicon carbide nanoparticles, ADVANCED ENGINEERING MATERIALS **7**, 937–945 (2005).

[65] M. Müller and K. Albe, Lattice Monte Carlo simulations of FePt nanoparticles: influence of size, composition, and surface segregation on order-disorder phenomena, PHYSICAL REVIEW B **72** (2005) 10.1103/PhysRevB.72.094203.

[66] P. Erhart and K. Albe, The role of thermostats in modeling vapor phase condensation of silicon nanoparticles, APPLIED SURFACE SCIENCE **226**, 12–18 (2004).

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Battery Materials

[69] A. Gautam, M. Sadowski, N. Prinz, H. Eickhoff, N. Minafra, M. Ghidiu, S. P. Culver, K. Albe, T. F. Faessler, M. Zobel, and W. G. Zeier, Rapid crystallization and kinetic freezing of site-disorder in the lithium superionic argyrodite Li_6PS_5Br, CHEMISTRY OF MATERIALS **31**, 10178–10185 (2019).

[70] P. Stein, A. Moradabadi, M. Diehm, B.-X. Xu, and K. Albe, The influence of anisotropic surface stresses and bulk stresses on defect thermodynamics in $LiCoO_2$ nanoparticles, ACTA MATERIALIA **159**, 225–240 (2018).

[71] M. Sadowski, S. Sicolo, and K. Albe, Defect thermodynamics and interfacial instability of crystalline $Li_4P_2S_6$, SOLID STATE IONICS **319**, 53–60 (2018).

[72] S. Sicolo, C. Kalcher, S. J. Sedlmaier, J. Janek, and K. Albe, Diffusion mechanism in the superionic conductor Li_4PS_4I studied by first-principles calculations, SOLID STATE IONICS **319**, 83–91 (2018).

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[74] M. Lepple, J. Rohrer, R. Adam, D. M. Cupid, D. Rafaja, K. Albe, and H. J. Seifert, Thermochemical stability of Li-Cu-O ternary compounds stable at room temperature analyzed by experimental and theoretical methods, INTERNATIONAL JOURNAL OF MATERIALS RESEARCH **108**, 959–970 (2017).

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[76] J. Rohrer, D. Vrankovic, D. Cupid, R. Riedel, H. J. Seifert, K. Albe, and M. Graczyk-Zajac, Si- and sn-containing SiOCN-based nanocomposites as anode materials for lithium ion batteries: synthesis, thermodynamic characterization and modeling, INTERNATIONAL JOURNAL OF MATERIALS RESEARCH **108**, 920–932 (2017).

[77] M. Fingerle, R. Buchheit, S. Sicolo, K. Albe, and R. Hausbrand, Reaction and space charge layer formation at the $LiCoO_2 - LiPON$ interface: insights on defect formation and ion energy level alignment by a combined surface science simulation approach, CHEMISTRY OF MATERIALS **29**, 7675–7685 (2017).

[78] S. Sicolo, M. Fingerle, R. Hausbrand, and K. Albe, Interfacial instability of amorphous LiPON against lithium: a combined density functional theory and spectroscopic study, JOURNAL OF POWER SOURCES **354**, 124–133 (2017).

[79] C. Dietrich, M. Sadowski, S. Sicolo, D. A. Weber, S. J. Sedlmaier, K. S. Weldert, S. Indris, K. Albe, J. Janek, and W. G. Zeier, Local structural investigations, defect formation, and ionic conductivity of the lithium ionic conductor $Li_4P_2S_6$, CHEMISTRY OF MATERIALS **28**, 8764–8773 (2016).

[80] S. Sicolo and K. Albe, First-principles calculations on structure and properties of amorphous $Li_5P_4O_8N_3$ (LiPON), JOURNAL OF POWER SOURCES **331**, 382–390 (2016).

[81] J. Rohrer, A. Moradabadi, K. Albe, and P. Kaghazchi, On the origin of anisotropic lithiation of silicon, JOURNAL OF POWER SOURCES **293**, 221–227 (2015).

[82] R. Hausbrand, G. Cherkashinin, H. Ehrenberg, M. Gr"oting, K. Albe, C. Hess, and W. Jaegermann, Fundamental degradation mechanisms of layered oxide Li-ion battery cathode materials: methodology, insights and novel approaches, MATERIALS SCIENCE AND ENGINEERING B-ADVANCED FUNCTIONAL SOLID-STATE MATERIALS **192**, 3–25 (2015).

[83] J. Rohrer and K. Albe, Insights into degradation of si anodes from first-principle calculations, JOURNAL OF PHYSICAL CHEMISTRY C **117**, 18796–18803 (2013).

Photovoltaic Absorbers and Buffer Materials

[84] E. Ghorbani, D. Barragan-Yani, and K. Albe, Towards intermediate-band photovoltaic absorbers: theoretical insights on the incorporation of Ti and Nb in In_2S_3, NPJ COMPUTATIONAL MATERIALS **6** (2020) 10.1038/s41524-020-00350-2.

[85] C. Li, E. S. Sanli, D. Barragan-Yani, H. Stange, M.-D. Heinemann, D. Greiner, W. Sigle, R. Mainz, K. Albe, D. Abou-Ras, and P. A. van Aken, Secondary-phase-assisted grain boundary migration in $CuInSe_2$, PHYSICAL REVIEW LETTERS **124** (2020) 10.1103/PhysRevLett.124.095702.

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