André Schleife
Associate Professor

Department of Materials Science and Engineering
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Professional Preparation

10/2006 – 06/2010: Ph.D. student (mentor Prof. Dr. Friedhelm Bechstedt), Friedrich-Schiller-University Jena, Germany
Dr. rer. nat. (Ph.D. in physics); grade: summa cum laude
Thesis: "Exciting Imperfection—Real-structure effects in magnesium-, cadmium-, and zinc-oxide";

10/2004 – 09/2006: Friedrich-Schiller-University Jena, Germany
University Diploma (M.Sc.);

10/2001 – 09/2004: Technical University Chemnitz, Germany

Appointments

08/2020 – current: Blue Waters Associate Professor, Department of Materials Science and Engineering, University of Illinois at Urbana-Champaign

12/2013 – 08/2020: Blue Waters Assistant Professor, Department of Materials Science and Engineering, University of Illinois at Urbana-Champaign

02/2011 – 12/2013: Directorate Postdoctoral researcher in the "Quantum Simulations Group", Lawrence Livermore National Laboratory, Livermore, California, USA

07/2010 – 01/2011: Postdoctoral researcher in the "Condensed Matter Theory Group", Friedrich-Schiller-University Jena, Germany

03/2008 – 06/2008: Research visit (mentor: Prof. Dr. Chris Van de Walle), University of California, Santa Barbara, USA

09/2004: Student researcher in the "Spectrométries et Dynamique Moléculaire" group, Université de Provence, Marseille, France

03/2004 – 04/2004: Student researcher in the "Ion-beam analytics" group, Forschungszentrum Rossendorf, Germany

02/2002 – 12/2004: Student researcher in the "Optical spectroscopy and molecular physics" group, Technical University Chemnitz, Germany

Awards, Recognition, Fellowships

Research

08/2020: Mercator Fellow for the SFB 1242

01/2019: Finalist "Rising Stars in Computational Materials Science"

03/2018: Office of Naval Research (ONR) Young Investigator Award

09/2017: ACS PRF 2017 Doctoral New Investigator

07/2017: National Center for Supercomputing Applications Faculty Fellowship

02/2016: National Science Foundation (NSF) CAREER Award

09/2012: LLNL Physical and Life Sciences Directorate Outstanding Postdoc Award

07/2012: LLNL Physical and Life Sciences Directorate Poster Award

10/2010: "Young Scientist Best Poster Presentation Award" at the 3rd International Symposium on Transparent Conductive Materials, Analipsi, Greece

06/2007: Heptagon "Sven-Bühling" prize

Teaching

05/2017: List of Teachers Ranked as Excellent by their Students for MSE304-Electronic Properties of Materials

12/2018: List of Teachers Ranked as Excellent by their Students for MSE404-Computational MSE

05/2019: List of Teachers Ranked as Excellent by their Students for MSE304-Electronic Properties of Materials

12/2019: List of Teachers Ranked as Excellent by their Students for MSE404-Computational MSE

05/2020: List of Teachers Ranked as Excellent by their Students for MSE304-Electronic Properties of Materials

Professional Activities

Editorial and Advisory Activities

2019 – current: Editor Materials Science in Semiconductor Processing

2018 – current: Elected Member of the American Physical Society, Division of Computational Physics (DCOMP) Executive Committee

2017 – current: Member of the DCOMP Program Committee for the APS March Meeting

2018 – current: Editorial Board member "Electronic Structure" (IOP Journal)

2017 – current: Editorial Board member Journal of Physics: Condensed Matter (IOP Journal)

2014 – 2018: Member of the SPIE Information Technology Committee

Outreach Activities

2012 – 2018: Outreach to High-School students in the "Adopt-a-Physicist" program of the physics honor society "Sigma Pi Sigma"

2015 – 2018: High-school student outreach within "Upward Bound"

2015 – current: Contributor to "Girls Learning About Materials" Summer Camp

2018 – current: Engineering Open House contribution "Virtual Reality and Ray Tracing for Materials Science"

2014 – current: Research Mentor for the Students Pushing for Innovation program (14 students total)

2018 – current: Research Mentor for the Uni High Frankel Scholar Program for High-school students (3 students total)

2017 – current: Research Mentor for the Research Experiences for Undergraduates (REU) "INCLUSION" program (7 students total)

2012 – 2013: News contributor "Materials Views", Wiley Publishing Company

Organization of Conferences and Workshops

2020: Co-organizer of a Tutorial on "Data Analysis and Modern Visualization", Invited Symposium on "Toward Precise Ab Initio Simulations of the Ultrafast Dynamics of Electrons and Phonons", and Focus Topic on "First-principles Modeling of Excited-State Phenomena in Materials", APS March Meeting 2020, Denver, CO

2019: Co-organizer of "School and Workshop on Time-Dependent Density Functional Theory", Rutgers, NJ

2019: Co-organizer of "Recent Developments in Electronic Structure", Urbana, IL

2018: Co-organizer of a Tutorial on "First-Principles Techniques for Interacting Electrons and Phonons", and Focus Topic on "First-principles Modeling of Excited-State Phenomena in Materials", APS March Meeting 2019, Boston, MA

2018: Member of the Technical Program Sub-Committee on "Semiconductor physics", Compound Semiconductor Week 2018, Boston, MA

2018: Co-organizer of a Mini Symposium on "Large Scale Electronic-Structure Calculations on Modern and Future High-Performance Supercomputers", Platform for Advanced Scientific Computing (PASC) Conference, Basel, Switzerland

2018: Co-organizer of an Invited Session on "Simulating Magnetization Switching Across Multiple Time and Length Scales" and Focus Topic on "First-Principles Modeling of Excited-State Phenomena in Materials", APS March Meeting 2018, Los Angeles, CA

07/2017 Co-organizer of "Telluride School and Workshop on Time-Dependent Density Functional Theory", Telluride, CO

2017: Co-organizer of an Invited Session on "Predictive Modeling of Electron-Phonon Coupling in Condensed-Matter Physics ", Tutorial on "Electron Phonon Interactions", and Focus Topic on "First-Principles Modeling of Excited-State Phenomena in Materials", APS March Meeting 2017, New Orleans, LA

2016: Co-organizer of a Focus Topic on "Theory and Simulation of Excited-State Phenomena in Semiconductors and Nanostructures", APS March Meeting 2016, Baltimore, MD

2015: Co-organizer of a Focus Topic on "Theory and simulation of excited-state phenomena in semiconductors and nano structures", APS March Meeting 2015, San Antonio, TX

2012 – 2013: Co-organizer and proceedings editor for the symposium "Oxide Semiconductors", Fall Meeting of the Materials Research Society 2012, Boston, USA

Short Courses

08/2019 Organizer and teacher: "Summer School and Workshop on Time-Dependent Density Functional Theory", Rutgers, NJ

06/2019 Organizer and teacher: Two-week class on "First-principles Quantum Simulations" at UFABC, São Paulo within the Brazil-U.S. Professorship/Lectureship Program of the American Physical Society

07/2017 Organizer and teacher: "Telluride School on Time-Dependent Density Functional Theory", Telluride, CO

05/2017 Organizer and teacher: Two-week class on "Atomic Scale Simulations" at UFABC, São Paulo within the Brazil-U.S. Professorship/Lectureship Program of the American Physical Society

2014 Computational Chemistry And Materials Science Summer Institute, Lawrence Livermore National Lab: "Computational Methods for Atomistic Length and Time Scales" and "Quantum Interactions, Excited Electrons, and Their Real-Time Dynamics"

Reviewer

Proposals Department of Energy, National Science Foundation, Deutsche Forschungsgemeinschaft, Blue Waters Project, Research Corporation for Scientific Advancement, National Center for Supercomputing Applications, CSCS Swiss National Supercomputing Centre, Wiley Publishing Company, Springer

Journals e.g. Nature Materials, Nature Communications, Science Advances, Physical Review Letters, Physical Review B, Physical Review Applied, Advanced Energy Materials, Nano Letters, Journal of the American Chemical Society, The Journal of Chemical Physics, Applied Physics Letters, Physical Chemistry Chemical Physics, Journal of Physics: Condensed Matter, Scientific Reports, Journal of Applied Physics, Journal of Materials Research, Journal of Materials Science, Physica Status Solidi B, International Journal of Quantum Chemistry, Journal of Physics and Chemistry of Solids, Journal of Alloys and Compounds, Computational Materials Science, Computational and Theoretical Chemistry, Optical Materials, Microelectronic Engineering, Physica B, Superlattices and Microstructures, Materials Chemistry and Physics, The European Physical Journal B, Journal of Luminescence, Journal of Electronic Materials, Journal of Photovoltaics, Journal of the Optical Society of America B, Journal of Solid State Chemistry, Journal of Raman Spectroscopy

Member

- American Physical Society
- American Chemical Society
- German Physical Society
- Materials Research Society
- Research Team Leader, European Theoretical Spectroscopy Facility

PhD students

- Xiao Zhang (graduated)
- Josh Leveillee (graduated)
- Cheng-Wei Lee (graduated)
- Ethan Shapera (passed preliminary exam)

- Alina Kononov (graduated)
- Kisung Kang (passed preliminary exam)
- Erick Hernandez
- Yifan Yao
- Brian Robinson
- Gillian Nolan
- Junehu Park
- Cindy Wong

Postdocs

- Tatiane Pereira dos Santos

Links

Homepage: http://schleife.matse.illinois.edu/

Google Scholar: http://scholar.google.com/citations?user=LQLGI5sAAAAJ

Linked-In: http://www.linkedin.com/pub/andr%C3%A9-schleife/2b/78/603

Twitter: @aschleife

Peer Reviewed Journal Publications [*h* index (Google Scholar): 32]

[98] M. H. Karigerasi, K. Kang, G. E. Granroth, A. Banerjee, **A. Schleife**, and D. P. Shoemaker: Strongly two-dimensional exchange interactions in the in-plane metallic antiferromagnet Fe_2As probed by inelastic neutron scattering. In: *Phys. Rev. Materials* **4**, p. 114416 (2020).

[97] K. Yang, K. Kang, Z. Diao, M. H. Karigerasi, D. P. Shoemaker, **A. Schleife**, and D. G. Cahill: Magnetocrystalline anisotropy of the easy-plane metallic antiferromagnet Fe_2As. In: *Phys. Rev. B* **102**, p. 064415 (2020).

[96] A. Kononov and **A. Schleife**: Pre-equilibrium stopping and charge capture in proton-irradiated aluminum sheets. In: *Phys. Rev. B* **102**, p. 165401 (2020).

[95] S. Richter, O. Herrfurth, S. Espinoza, M. Rebarz, M. Kloz, J. A. Leveillee, **A. Schleife**, S. Zollner, M. Grundmann, J. Andreasson, and R. Schmidt-Grund: Ultrafast dynamics of hot charge carriers in an oxide semiconductor probed by femtosecond spectroscopic ellipsometry. In: *New J. Phys.* **22**, p. 083066 (2020).

[94] C.-W. Lee, J. A. Stewart, R. Dingreville, S. M. Foiles, and **A. Schleife**: Multiscale simulations of electron and ion dynamics in self-irradiated silicon. In: *Phys. Rev. B* **102**, p. 024107 (2020).

[93] C.-H. Lee, A. Khan, D. Luo, T. P. Santos, C. Shi, B. E. Janicek, S. Kang, W. Zhu, N. A. Sobh, **A. Schleife**, B. K. Clark, and P. Y. Huang: Deep Learning Enabled Strain Mapping of Single-Atom Defects in Two-Dimensional Transition Metal Dichalcogenides with Sub-Picometer Precision. In: *Nano Lett.* **20**, pp. 3369–3377 (2020).

[92] A. Bhutani, X. Zhang, P. Behera, R. Thiruvengadam, S. E. Murray, **A. Schleife**, and D. P. Shoemaker: New Family of Anisotropic Zinc-Based Semiconductors in a Shallow Energy Landscape. In: *Chem. Mater.* **32**, pp. 326–332 (2020).

[91] K. Yang, K. Kang, Z. Diao, A. Ramanathan, M. H. Karigerasi, D. P. Shoemaker, **A. Schleife**, and D. G. Cahill: Magneto-optic response of the metallic antiferromagnet Fe_2As to ultrafast temperature excursions. In: *Phys. Rev. Materials* **3**, p. 124408 (2019).

[90] M. H. Karigerasi, K. Kang, A. Ramanathan, D. L. Gray, M. D. Frontzek, H. Cao, **A. Schleife**, and D. P. Shoemaker: In-plane hexagonal antiferromagnet in the Cu-Mn-As system $Cu_{0.82}Mn_{1.18}As$. In: *Phys. Rev. Materials* **3**, p. 111402 (2019).

[89] J. Leveillee, C. Katan, J. Even, D. Ghosh, W. Nie, A. D. Mohite, S. Tretiak, **A. Schleife**, and A. J. Neukirch: Tuning Electronic Structure in Layered Hybrid Perovskites with Organic Spacer Substitution. In: *Nano Lett.* **19**, pp. 8732–8740 (2019).

[88] B. A. Thurston, E. P. Shapera, J. D. Tovar, **A. Schleife**, and A. L. Ferguson: Revealing the Sequence-Structure-Electronic Property Relation of Self-Assembling π-Conjugated Oligopeptides by Molecular and Quantum Mechanical Modeling. In: *Langmuir* **35**, pp. 15221–15231 (2019).

[87] J. Leveillee and **A. Schleife**: Free-electron effects on the optical absorption of the hybrid perovskite $CH_3NH_3PbI_3$ from first principles. In: *Phys. Rev. B* **100**, p. 035205 (2019).

[86] C.-W. Lee and **A. Schleife**: Hot-Electron-Mediated Ion Diffusion in Semiconductors for Ion-Beam Nanostructuring. In: *Nano Lett.* **19**, pp. 3939–3947 (2019).

[85] A. J. Martinolich, C.-W. Lee, I.-T. Lu, S. C. Bevilacqua, M. B. Preefer, M. Bernardi, **A. Schleife**, and K. A. See: Solid-State Divalent Ion Conduction in $ZnPS_3$. In: *Chem. Mater.* **31**, pp. 3652–3661 (2019).

[84] C. Wagner, J. Schuster, and **A. Schleife**: Strain and screening: Optical properties of a small-diameter carbon nanotube from first principles. In: *Phys. Rev. B* **99**, p. 075140 (2019).

[83] D. Li, A. Schleife, D. G. Cahill, G. Mitchson, and D. C. Johnson: Ultralow shear modulus of incommensurate $[SnSe]_n[MoSe_2]_n$ layers synthesized by the method of modulated elemental reactants. In: *Phys. Rev. Materials* **3**, p. 043607 (2019).

[82] E. P. Shapera and **A. Schleife**: Database-Driven Materials Selection for Semiconductor Heterojunction Design. In: *Adv. Theor. Sim.* **1**, p. 1800075 (2018).

[81] J. Leveillee, C. Katan, L. Zhou, A. D. Mohite, J. Even, S. Tretiak, **A. Schleife**, and A. J. Neukirch: Influence of Pi-conjugated cations and halogen substitution on the optoelectronic and excitonic properties of layered hybrid perovskites. In: *Phys. Rev. Materials* **2**, p. 105406 (2018).

[80] **A. Schleife**, M. D. Neumann, N. Esser, Z. Galazka, A. Gottwald, J. Nixdorf, R. Goldhahn, and M. Feneberg: Optical properties of In_2O_3 from experiment and first-principles theory: influence of lattice screening. In: *New J. Phys.* **20**, p. 053016 (2018).

[79] Y.-C. Chen, I. Ghosh, **A. Schleife**, P. S. Carney, and G. Bahl: Optimization of anisotropic photonic density of states for Raman cooling of solids. In: *Phys. Rev. A* **97**, p. 043835 (2018).

[78] Y. Kim, K. Kang, **A. Schleife**, and M. J. Gilbert: Voltage-induced switching of an antiferromagnetically ordered topological Dirac semimetal. In: *Phys. Rev. B* **97**, p. 134415 (2018).

[77] X. Zhang and **A. Schleife**: Nonequilibrium BN-ZnO: Optical properties and excitonic effects from first principles. In: *Phys. Rev. B* **97**, p. 125201 (2018).

[76] M.-F. Lin, M. A. Verkamp, J. Leveillee, E. S. Ryland, K. Benke, K. Zhang, C. Weninger, X. Shen, R. Li, D. Fritz, U. Bergmann, X. Wang, **A. Schleife**, and J. Vura-Weis: Carrier-Specific Femtosecond XUV Transient Absorption of PbI_2 Reveals Ultrafast Nonradiative Recombination. In: *J. Phys. Chem. C* **121** (50), pp. 27886–27893 (2017).

[75] E. W. Draeger, X. Andrade, J. A. Gunnels, A. Bhatele, **A. Schleife**, and A. A. Correa: Massively parallel first-principles simulation of electron dynamics in materials. In: *J. Parallel Distr. Com.* **106**, pp. 205–214 (2017).

[74] S. J. Lim, **A. Schleife**, and A. M. Smith: Optical determination of crystal phase in semiconductor nanocrystals. In: *Nat. Commun.* **8**, p. 14849 (2017).

[73] G.-M. Choi, **A. Schleife**, and D. G. Cahill: Optical-helicity-driven magnetization dynamics in metallic ferromagnets. In: *Nat. Commun.* **8**, p. 15085 (2017).

[72] R. D. McAuliffe, C. A. Miller, X. Zhang, B. S. Hulbert, A. Huq, C. dela Cruz, **A. Schleife**, and D. P. Shoemaker: Structural, Electronic, and Optical Properties of K2Sn3O7 with an Offset Hollandite Structure. In: *Inorg. Chem.* **56**, pp. 2914–2918 (2017).

[71] **A. Schleife**, X. Zhang, Q. Li, P. Erhart, and D. Åberg: Excitons in scintillator materials: Optical properties and electron-energy loss spectra of NaI, $LaBr_3$, BaI_2, and SrI_2. In: *J. Mater. Res.* **32**, pp. 1–8 (2017).

[70] J.-X. Shen, **A. Schleife**, A. Janotti, and C. G. Van de Walle: Effects of La 5d and 4f states on the electronic and optical properties of LaAlO3. In: *Phys. Rev. B* **94**, p. 205203 (2016).

[69] A. Lim, W. M. C. Foulkes, A. P. Horsfield, D. R. Mason, **A. Schleife**, E. W. Draeger, and A. A. Correa: Electron Elevator: Excitations across the Band Gap via a Dynamical Gap State. In: *Phys. Rev. Lett.* **116**, p. 043201 (2016), Editor's suggestion.

[68] S. J. Lim, L. Ma, **A. Schleife**, and A. M. Smith: Quantum dot surface engineering: Toward inert fluorophores with compact size and bright, stable emission. In: *Coord. Chem. Rev.* **320–321**, pp. 216–237 (2016).

[67] R. Mansbach, A. Ferguson, K. Kilian, J. Krogstad, C. Leal, **A. Schleife**, D. R. Trinkle, M. West, and G. L. Herman: Reforming an undergraduate materials science curriculum with computational modules. In: *J. Materials Education* **38**, pp. 161–174 (2016).

[66] **A. Schleife**, Y. Kanai, and A. A. Correa: Accurate atomistic first-principles calculations of electronic stopping. In: *Phys. Rev. B* **91**, p. 014306 (2015).

[65] A. McAllister, D. Åberg, **A. Schleife**, and E. Kioupakis: Auger recombination in sodium-iodide scintillators from first principles. In: *Appl. Phys. Lett.* **106** (14), p. 141901 (2015).

[64] P. Erhart, B. Sadigh, **A. Schleife**, and D. Åberg: First-principles study of codoping in lanthanum bromide. In: *Phys. Rev. B* **91**, p. 165206 (2015).

[63] K. G. Reeves, **A. Schleife**, A. A. Correa, and Y. Kanai: Role of Surface Termination on Hot Electron Relaxation in Silicon Quantum Dots: A First-Principles Dynamics Simulation Study. In: *Nano Lett.* **15** (10), pp. 6429–6433 (2015).

[62] D. Åberg, B. Sadigh, **A. Schleife**, and P. Erhart: Origin of resolution enhancement by co-doping of scintillators: Insight from electronic structure calculations. In: *Appl. Phys. Lett.* **104** (21) (2014).

[61] C. Rödl and **A. Schleife**: Photoemission spectra and effective masses of *n*- and *p*-type oxide semiconductors from first principles: ZnO, CdO, SnO2, MnO, and NiO. In: *Phys. Status Solidi A* **211** (1), pp. 74–81 (2014).

[60] P. Erhart, **A. Schleife**, B. Sadigh, and D. Åberg: Quasiparticle spectra, absorption spectra, and excitonic properties of NaI and SrI_2 from many-body perturbation theory. In: *Phys. Rev. B* **89**, p. 075132 (2014).

[59] L. C. de Carvalho, **A. Schleife**, J. Furthmüller, and F. Bechstedt: Ab-initio calculation of optical properties of wurtzitic $In_xGa_{1-x}N$ and $In_xAl_{1-x}N$ alloys including excitonic effects. In: *Phys. Rev. B* **87**, p. 195211 (2013).

[58] J. B. Varley, **A. Schleife**, A. Janotti, and C. G. Van de Walle: Ambipolar doping in SnO. In: *Appl. Phys. Lett.* **103** (8), p. 082118 (2013).

[57] M. R. Wagner, G. Callsen, J. S. Reparaz, R. Kirste, A. Hoffmann, A. V. Rodina, **A. Schleife**, F. Bechstedt, and M. R. Phillips: Effects of strain on the valence band structure and exciton-polariton energies in ZnO. In: *Phys. Rev. B* **88**, p. 235210 (2013).

[56] **A. Schleife**, P. Rinke, F. Bechstedt, and C. G. Van de Walle: Enhanced Optical Absorption Due to Symmetry Breaking in $TiO_{2(1-x)}S_{2x}$ Alloys. In: *J. Phys. Chem. C* **117**, pp. 4189–4193 (2013).

[55] B. Höffling, **A. Schleife**, C. Rödl, and F. Bechstedt: Band discontinuities at Si-TCO interfaces from quasiparticle calculations: Comparison of two alignment approaches. In: *Phys. Rev. B* **85**, p. 035305 (2012).

[54] J. Furthmüller, F. Hachenberg, **A. Schleife**, D. Rogers, F. H. Teherani, and F. Bechstedt: Clustering of N impurities in ZnO. In: *Appl. Phys. Lett.* **100**, p. 022107 (2012).

[53] L. C. de Carvalho, **A. Schleife**, J. Furthmüller, and F. Bechstedt: Distribution of cations in wurtzitic $In_xGa_{1-x}N$ and $In_xAl_{1-x}N$ alloys: Consequences for energetics and quasiparticle electronic structures. In: *Phys. Rev. B* **85**, p. 115121 (2012).

[52] S. Küfner, **A. Schleife**, B. Höffling, and F. Bechstedt: Energetics and approximate quasiparticle electronic structure of low-index surfaces of SnO_2. In: *Phys. Rev. B* **86**, p. 075320 (2012).

[51] P. Rinke, **A. Schleife**, E. Kioupakis, A. Janotti, C. Rödl, F. Bechstedt, M. Scheffler, and C. G. Van de Walle: First-Principles Optical Spectra for F Centers in MgO. In: *Phys. Rev. Lett.* **108**, p. 126404 (2012).

[50] **A. Schleife**, E. W. Draeger, Y. Kanai, and A. A. Correa: Plane-wave pseudopotential implementation of explicit integrators for time-dependent Kohn-Sham equations in large-scale simulations. In: *J. Chem. Phys.* **137** (22), 22A546 (2012).

[49] A. Kronenberger, A. Polity, D. M. Hofmann, B. K. Meyer, **A. Schleife**, and F. Bechstedt: Structural, electrical, and optical properties of hydrogen-doped ZnO films. In: *Phys. Rev. B* **86**, p. 115334 (2012).

[48] A. Belabbes, L. C. de Carvalho, **A. Schleife**, and F. Bechstedt: Cubic inclusions in hexagonal AlN, GaN, and InN: Electronic states. In: *Phys. Rev. B* **84**, p. 125108 (2011).

[47] L. C. de Carvalho, **A. Schleife**, and F. Bechstedt: Influence of exchange and correlation on structural and electronic properties of AlN, GaN, and InN polytypes. In: *Phys. Rev. B* **84**, p. 195105 (2011).

[46] A. Riefer, F. Fuchs, C. Rödl, **A. Schleife**, F. Bechstedt, and R. Goldhahn: Interplay of excitonic effects and van Hove singularities in optical spectra: CaO and AlN polymorphs. In: *Phys. Rev. B* **84**, p. 075218 (2011).

[45] **A. Schleife**, C. Rödl, F. Fuchs, K. Hannewald, and F. Bechstedt: Optical Absorption in Degenerately Doped Semiconductors: Mott Transition or Mahan Excitons?, in: *Phys. Rev. Lett.* **107**, p. 236405 (2011).

[44] **A. Schleife**, J. B. Varley, F. Fuchs, C. Rödl, F. Bechstedt, P. Rinke, A. Janotti, and C. G. Van de Walle: Tin dioxide from first principles: Quasiparticle electronic states and optical properties. In: *Phys. Rev. B* **83**, p. 035116 (2011).

[43] **A. Schleife**, M. Eisenacher, C. Rödl, F. Fuchs, J. Furthmüller, and F. Bechstedt: Ab initio description of heterostructural alloys: Thermodynamic and structural properties of $Mg_x\,Zn_{1-x}\,O$ and $Cd_xZn_{1-x}O$. In: *Phys. Rev. B* **81**, p. 245210 (2010).

[42] B. Höffling, **A. Schleife**, F. Fuchs, C. Rödl, and F. Bechstedt: Band lineup between silicon and transparent conducting oxides. In: *Appl. Phys. Lett.* **97**, p. 032116 (2010).

[41] E. Kioupakis, P. Rinke, **A. Schleife**, F. Bechstedt, and C. G. Van de Walle: Free-carrier absorption in nitrides from first principles. In: *Phys. Rev. B* **81**, p. 241201 (2010).

[40] L. C. de Carvalho, **A. Schleife**, F. Fuchs, and F. Bechstedt: Valence-band splittings in cubic and hexagonal AlN, GaN, and InN. In: *Appl. Phys. Lett.* **97**, p. 232101 (2010).

[39] **A. Schleife**, F. Fuchs, C. Rödl, J. Furthmüller, and F. Bechstedt: Band-structure and optical-transition parameters of wurtzite MgO, ZnO, and CdO from quasiparticle calculations. In: *Phys. Status Solidi B* **246**, pp. 2150–2153 (2009).

[38] **A. Schleife**, F. Fuchs, C. Rödl, J. Furthmüller, and F. Bechstedt: Branch-point energies and band discontinuities of III-nitrides and III-/II-oxides from quasiparticle band-structure calculations. In: *Appl. Phys. Lett.* **94**, p. 012104 (2009).

[37] **A. Schleife**, C. Rödl, F. Fuchs, J. Furthmüller, and F. Bechstedt: Optical and energy-loss spectra of MgO, ZnO, and CdO from ab initio many-body calculations. In: *Phys. Rev. B* **80**, p. 035112 (2009).

[36] P. D. C. King, T. D. Veal, **A. Schleife**, J. Zúñiga-Pérez, B. Martel, P. H. Jefferson, F. Fuchs, V. Muñoz-Sanjosé, F. Bechstedt, and C. F. McConville: Valence-band electronic structure of CdO, ZnO, and MgO from x-ray photoemission spectroscopy and quasi-particle-corrected density-functional theory calculations. In: *Phys. Rev. B* **79**, p. 205205 (2009).

[35] **A. Schleife**, C. Rödl, F. Fuchs, J. Furthmüller, F. Bechstedt, P. H. Jefferson, T. D. Veal, C. F. McConville, L. F. J. Piper, A. DeMasi, K. E. Smith, H. Lösch, R. Goldhahn, C. Cobet, J. Zúñiga-Pérez, and V. Muñoz-Sanjosé: *Ab-initio* Studies of Electronic and Spectroscopic Properties of MgO, ZnO, and CdO. In: *J. Korean Phys. Soc.* **53**, pp. 2811–2815 (2008).

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[18] **A. Schleife**, E. W. Draeger, V. M. Anisimov, A. A. Correa, and Y. Kanai: Quantum Dynamics Simulation of Electrons in Materials on High-Performance Computers. In: *Comput. Sci. Eng.* **16** (5), pp. 54–60 (2014), Special Issue on Advances in Leadership Computing.

[17] **A. Schleife** and F. Bechstedt: Ab initio description of quasiparticle band structures and optical near-edge absorption of transparent conducting oxides. In: *J. Mater. Res.* **27**, pp. 2180–2189 (2012), Focus Issue: Oxide Semiconductors.

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Cover stories, Conference proceedings (Not peer reviewed)

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Books or book chapters (Not peer reviewed)

[10] E. Shapera and **A. Schleife**: *Blue Waters: Sustained Petascale In Action: Enabling Transformative Research, 2019 Annual Report*. National Center for Supercomputing Applications, 2019, chap. Discovery of new plasmonic materials via high throughput machine learning.

[9] A. Kononov and **A. Schleife**: *Blue Waters: Sustained Petascale In Action: Enabling Transformative Research, 2019 Annual Report*. National Center for Supercomputing Applications, 2019, chap. Ion-irradiated 2D Materials.

[8] A. Kononov and **A. Schleife**: *Blue Waters: Sustained Petascale In Action: Enabling Transformative Research, 2018 Annual Report*. National Center for Supercomputing Applications, 2018, chap. Electron Dynamics of Ion-irradiated Graphene.

[7] K. Kang and **A. Schleife**: *Blue Waters: Sustained Petascale In Action: Enabling Transformative Research, 2018 Annual Report*. National Center for Supercomputing Applications, 2018, chap. Magneto-optical Kerr effect of antiferromagnetic materials in external magnetic fields.

[6] A. S. **A. Schleife** Sung Jun Lim: *Blue Waters: Sustained Petascale In Action: Enabling Transformative Research, 2017 Annual Report*. National Center for Supercomputing Applications, 2017, chap. Optical Determination of Crystal Phase in Semiconductor Nanocrystals.

[5] A. Kononov and **A. Schleife**: *Blue Waters: Sustained Petascale In Action: Enabling Transformative Research, 2016 Annual Report*. National Center for Supercomputing Applications, 2016, chap. Non-Adiabatic Ultrafast Electron-Ion Dynamics Near Aluminum Surfaces.

[4] J. Leveillee and **A. Schleife**: *Blue Waters: Sustained Petascale In Action: Enabling Transformative Research, 2016 Annual Report*. National Center for Supercomputing Applications, 2016, chap. Lattice screening and optical properties of novel perovskite photovoltaic materials.

[3] **A. Schleife** and J. Varley: *Blue Waters: Sustained Petascale In Action: Enabling Transformative Research, 2015 Annual Report*. National Center for Supercomputing Applications, 2015, chap. Theoretical Spectroscopy for Transparent Conducting Oxides, ISBN: 9780990838524.

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[1] **A. Schleife**: *Electronic and optical properties of MgO, ZnO, and CdO*. Südwestdeutscher Verlag für Hochschulschriften, 2011, ISBN: 3838127668.

Invited Talks and Colloquia

68. **"Electronic excitations: Optical properties, femto-second dynamics, and materials selection"**; University of California, Riverside (2020)
67. **"Optical properties, dielectric screening, and heterojunction design for oxides and chalcogenides"**; Electronic Materials and Applications 2020, Orlando FL (2020)
66. **"Electronic Excitations and Ultrafast Dynamics: Pushing Towards Materials Engineering and Design"**; 2020 TMS Annual Meeting & Exhibition, San Diego CA (2020)
65. **"Electronic excitations and ultrafast dynamics: First-principles simulations"**; 6th International Conference on Electronic Materials and Nanotechnology for Green Environment, Jeju Island, Korea (Virtual participation, 2020)
64. **"First-principles simulations of electronic excitations and real-time dynamics on high-performance super computers"**; APS March Meeting, Boston, MA (2019)
63. **"First-principles simulations of excited electronic states: Optical properties, particle radiation, and heterojunctions"**; ACS National Meeting, Orlando, FL (2019)
62. **"Ultrafast electron dynamics due to electronic stopping in bulk semiconductors"**; ACS National Meeting, Orlando, FL (2019)
61. **"Excited electronic states: Dielectric screening and hot-electron mediated ion diffusion"**; Northern Illinois University, DeKalb, IL (2019)
60. **"Electronic Response of Graphene to Ion Irradiation"**; Workshop on "Atomistic Simulations of Carbon-Based Materials", Helsinki, Finland (2019)
59. **"Excited electronic states and their ultrafast dynamics: Pushing towards materials engineering and design"**; UC Santa Barbara, Santa Barbara, CA (2019)
58. **"Hot-electron mediated ion diffusion and projectile-charge dynamics for radiation damage"**; Workshop on "Nonequilibrium Phenomena, Nonadiabatic Dynamics and Spectroscopy", Telluride CO (2019)
57. **"Hot-electron mediated ion diffusion and projectile-charge dynamics for radiation damage"**; Summer School and Workshop on Time-Dependent Density Functional Theory, Rutgers NJ (2019)
56. **"Excited electronic states: Dielectric screening and hot-electron mediated ion diffusion"**; Southern Illinois University, Carbondale IL (2019)
55. **"Excited electronic states and ultrafast dynamics: Pushing towards design of materials"**; ACS National Meeting, San Diego CA (2019)

54. **"Excited electrons in TCOs: Dielectric screening and electron dynamics"**; ACS National Meeting, TCO2019 - Conference on Transparent Conductive Oxides, Fundamentals and Applications, Leipzig, Germany (2019)
53. **"Excited electronic states: From femto-second dynamics to materials selection"**; UC Davis, Davis CA (2019)
52. **"Electronic excitations: Optical properties, femto-second dynamics, and materials selection"**; University Duisburg-Essen, Duisburg, Germany (2019)
51. **"Optical signatures of crystal phase: Bulk semiconductors and nanocrystals"**; Excited State Processes in Electronic and Bio Nanomaterials, Santa Fe, NM (2018)
50. **"Excitonic effects and dielectric screening in transparent conducting oxides"**; 14th International Ceramics Congress & 8th Forum on New Materials, Perugia, Italy (2018)
49. **"Excited-electron dynamics due to particle radiation in solids and near surfaces from time-dependent density-functional theory"**; ACS National Meeting, Boston, MA (2018)
48. **"Optical properties of materials: First-principles simulations and materials databases"**; Citrine Informatics, Redwood City, CA (2018)
47. **"Excited electrons in semiconductors: Dielectric screening and electron-ion dynamics"** Tyndall National Institute, Cork, Ireland (2018)
46. **"Excited electronic states: Dielectric screening and hot-electron mediated ion diffusion"**; Caltech, Pasadena, CA (2018)
45. **"Excited electronic states: Dielectric screening and hot-electron mediated ion diffusion"**; UC Berkeley (Computational Materials at Berkeley Seminar), Berkeley, CA (2018)
44. **"8th Workshop on Time-Dependent Density Functional Theory: Prospects and Applications"**; Benasque, Spain (2018)
43. **"Excited electronic states: Semiconductor heterojunctions and hot-electron mediated ion diffusion"**; LeHigh University, Bethlehem, PA (2018)
42. **"Optical properties of Ga_2O_3 from first principles: Excitons, Free carriers, and Dielectric screening"**; SPIE Photonics West, San Francisco CA (2018)
41. **"Excited electrons in semiconductors: Dielectric screening and non-adiabatic dynamics"**; University of California Santa Cruz, Santa Cruz CA (2018)
40. **"Excited-electron dynamics in time-dependent density functional theory: Particle radiation in solids, near defects, and surfaces "**; Argonne National Laboratory, Chicago IL (2017)
39. **"Electron-ion interaction in materials: Dielectric screening and non-adiabatic dynamics "**; International Center for Materials Nanoarchitectonics/NIMS, Tsukuba, Japan (2017)
38. **"Electron-ion interaction in materials: Dielectric screening and non-adiabatic dynamics "**; The University of Tokyo, Tokyo, Japan (2017)
37. **"Electron-ion interaction in materials: Dielectric screening and non-adiabatic dynamics "**; Colorado School of Mines, Golden CO (2017)
36. **"Electron-ion interaction in materials: Dielectric screening and non-adiabatic dynamics "**; University of Illinois at Chicago, Chicago IL (2017)
35. **"Excited electrons in semiconductors: Dielectric screening and non-adiabatic dynamics"**; Los

Alamos National Laboratory, Los Alamos NM (2017)

34. **"Electron-ion interaction: Dielectric screening and non-adiabatic dynamics in materials"**; Universidade Federal do ABC, Sao Paulo, Brazil (2017)

33. **"Electron-ion interaction: Dielectric screening and non-adiabatic dynamics in materials"**; Instituto de Física da USP, University of Sao Paulo, Sao Paulo, Brazil (2017)

32. **"Excited-electron dynamics near surfaces: Particle radiation in real-time TDDFT"**; Workshop on "Excited States: Electronic Structure and Dynamics", Telluride CO (2017)

31. **"Interaction of electrons and ions in materials: Dielectric screening and non-adiabatic dynamics"**; New Mexico State University, Las Cruces NM (2017)

30. **"Interaction of electrons and ions in materials: Dielectric screening and non-adiabatic dynamics"**; The University of Texas, El Paso TX (2017)

29. **"Accurate First-Principles Simulations of Excited Electrons and Ultrafast Electron-Ion Dynamics in Complex Materials"**; Sandia Special Seminar, Sandia National Laboratory (2016)

28. **"Accurate First-Principles Simulations of Excited Electrons and Ultrafast Electron-Ion Dynamics in Complex Materials"**; ARL Special Seminar, Army Research Laboratory (2016)

27. **"First-principles Simulations of Electronic Excitations and Ultrafast Real-time Dynamics in Semiconductors"**; Electronic Materials and Applications, Orlando FL (2016)

26. **"Quasiparticle energies, excitonic effects, and dielectric screening in transparent conducting oxides"**; APS March Meeting, Baltimore MD, (2016)

25. **"First-principles simulations of optical properties on the nanoscale"**; CNST 14th Annual Nanotechnology Workshop, Urbana IL (2016)

24. **"Theoretical spectroscopy of materials for oxide optoelectronics"**; Energy Materials Nanotechnology/Theory, Las Vegas NV (2016)

23. **"Particle radiation in real-time TDDFT: Massively parallel simulations of solids, defects, and surfaces"**; IBM Almaden, San Jose CA (2016)

22. **"Excited electrons in materials: Theoretical spectroscopy and real-time electron dynamics"**; Northrop Grumman Next, Redondo Beach CA (2016)

21. **"Quasiparticle energies, excitonic effects, and defects in optical materials"**; SAGE Electrochromics, Faribault MN (2016)

20. **"High-Performance Computing and Multi-Scale Simulations"**; Physics Department Colloquium, Technical University Chemnitz, Germany (2015)

19. **"High-Performance Computing and Multi-Scale Simulations"**; Dresden Center for Computational Materials Science, Technical University Dresden, Germany (2015)

18. **"Predictive First-principles Simulations of Excited Electrons and Ultrafast Electron-ion Dynamics in Complex Materials"**; Physics Department Colloquium, University of Missouri (2015)

17. **"Predictive First-principles Simulations of Excited Electrons and Ultrafast Electron-ion Dynamics in Complex Materials"**; Physics Department Colloquium, Case Western Reserve University (2015)

16. **"Predictive First-principles Simulations of Excited Electrons and Ultrafast Electron-ion Dynamics in Complex Materials"**; Materials Science and Engineering Department Colloquium, Binghamton University (2015)

15. **"Numerical integrators for a plane-wave implementation of real-time time-dependent density functional theory"**; Argonne Special Seminar, Argonne National Laboratory (2015)
14. **"*Ab-initio* description of the electronic stopping power beyond the Born-Oppenheimer approximation"**; University of Rochester, Rochester, USA (2012)
13. **"*Ab-initio* description of electronic and optical properties of transparent conductive oxides"**; University at Buffalo, Buffalo, USA (2012)
12. **"Theoretical prediction of physical properties of semiconducting oxides via ab-initio calculations"**; Workshop on "Novel Semiconducting Oxides", Berlin, Germany (2012)
11. **"Electronic and optical properties of transparent conductive oxides from *ab-initio* calculations"**; SPIE Photonics West, San Francisco, USA (2012)
10. **"Explicit integrators for the time-dependent Kohn-Sham equations"**; University of California Davis, Davis, USA (2011)
9. **"*Ab-initio* calculation of electronic and optical properties of transparent conductive oxides"**; Massachusetts Institute of Technology, Boston, USA (2011)
8. **"*Ab-initio* description of electronic and optical properties of transparent conductive oxides"**; Fall Meeting of the Materials Research Society, Boston, USA (2011)
7. **"*Ab-initio* calculation of electronic and optical properties of transparent conductive oxides"**; Spring meeting of the German Physical Society, Dresden, Germany (2011)
6. **"*Ab-initio* calculation of electronic and optical properties of transparent conductive oxides"**; Seminar within the Sonderforschungsbereich SFB 595, Technical University Darmstadt, Darmstadt, Germany (2011)
5. **"*Ab-initio* calculation of electronic and optical properties of transparent conductive oxides"**; University of York, York, United Kingdom (2010)
4. **"Electronic and optical properties of transparent conducting oxides and the influence of real-structure effects"**; Lawrence Livermore National Laboratory, Livermore, USA (2010)
3. **"Electronic and optical properties of transparent conducting oxides and the influence of real-structure effects"**; University of California, Berkeley, USA (2010)
2. **"Parameter-free description of electronic and optical properties of transparent conducting oxides"**; Focused workshop on semiconducting oxides, University of California, Santa Barbara, USA (2010)
1. **"From Ideal Bulk to Reality – Interplay of Excitonic Effects with Defects and Doping"**; 14th ETSF Workshop on Electronic Excitations, Evora, Portugal (2009)