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Education

- 08.2007 – 04.2011 Dr. rer. nat, *summa cum laude*
Leibniz Universität Hannover, Germany
Institut für Festkörperphysik (Prof. Herbert Pfnür)
· Adsorption of organic molecules on wide band-gap insulators
- 07.2005 – 08.2007 Research assistant, Fudan University
Institute of Microelectronic
· High-k dielectrics in nonvolatile memory
- 09.2002 – 07.2005 MSc. in Electrical Engineering, Fudan University
Institute of Microelectronics
· DFT study on atomic layer deposition of high-k gate dielectrics
- 09.1998 – 07.2002 BSc., Fudan University, Shanghai, China

Research Experience

- 06.2016 – present Post-doctoral researcher, UCLouvain, Belgium
Institute of Condensed Matter and Nanosciences
Profs. Gian-Marco Rignanese and Geoffroy Hautier
· Multicomponent alloys
· Emerging kesterite solar absorbers
· Many-body perturbation theory
· Nonempirical hybrid density functional
· High-throughput computational screening
- 04.2011 – 03.2016 Post-doctoral researcher, Ecole Polytechnique Fédérale de Lausanne (EPFL)
Chair of Atomic Scale Simulation
Prof. Alfredo Pasquarello
· Defects in semiconductors and insulators
· Interfaces in semiconductor heterojunctions
· Advanced electronic-structure methods: *GW* approximation and hybrid functionals
· Electronic structure of liquid water: many-body and nuclear quantum effects

Coding skills

FORTRAN, C, PYTHON, GNU BASH, MPI.

Active developer for [ABINIT](#) and [QUANTUM ESPRESSO](#).

Code developments

ABINIT	Bootstrap exchange-correlation kernel for accurate GW quasiparticle energies, Gygi-Baldereschi auxiliary function for the treatment of Coulomb singularity
QUANTUM-ESPRESSO	Range-separated hybrid density functional
FNV	PYTHON class for finite-size-corrections of periodic charged defects (https://github.com/wayn3/FNV)

Teaching Activities

03.2019 – 06.2019	Masters course: Atomistic and Nanoscopic Simulations Teaching assistance, UCLouvain
04.2012 – 04.2016	Masters course: Computational Simulation and Physical Systems I & II Teaching assistance, EPFL
06.2013 – 04.2014	Supervising a Masters student (Karim Steiner) Project: Band-offset of lattice matched semiconductor heterojunctions

Recent Talks and Seminars

05.2021	MRS Spring Meeting 2021 (virtual) Talk: “Origin of Low Conversion Efficiency of $\text{Cu}_2\text{ZnSnS}_4$ Kesterite Solar Absorber”
09.2018	Swiss Physics Society Annual Meeting 2018, Lausanne, Switzerland Invited talk: “Electronic structures through GW and hybrid functionals”
08.2017	29th International Conference on Defects in Semiconductors (ICDS), Matsue, Japan Invited talk: “Towards accurate determination of defect levels in semiconductors”
05.2017	ABINIT Developer Workshop 2017, Frèjus, France Invited talk: “Accurate band gaps via efficient vertex corrections in GW ”
10.2015	Université catholique de Louvain, Belgium Invited seminar: “Efficient vertex corrections in GW ”
09.2015	PSI- κ 2015 conference, San Sebastian, Spain Talk: “Accurate band gaps via efficient vertex corrections in GW ”
07.2015	International Conference on Defects in Semiconductors (ICDS 15), Espoo, Finland Talk: “Determination of defect energy levels through GW ”
04.2015	“Nothing is Perfect” workshop, Ascona, Switzerland Invited Talk: “First-principles determination of defect energy levels through GW ”
08.2014	International conference on the physics of semiconductors (ICPS 14), Austin, USA Talk: “Band offset of lattice-matched semiconductor heterojunctions”
07.2013	International Conference on Defects in Semiconductors (ICDS 13), Bologna, Italy Talk: “Defect energy levels: Hybrid functionals vs GW ”

Miscellaneous

Referee for *Phys. Rev. Lett.*, *Phys. Rev. B*, *Appl. Phys. Lett.*, *J. Phys. Chem. Lett.*, *J. Phys. Chem.*, *npj Comput. Mater.*

Publications in Chronological Order

- [1] G. Bokas, W. Chen, A. Hilhorst, P. Jacques, S. Gorsse, and G. Hautier, “Unveiling the thermodynamic driving forces for high entropy alloys formation through big data ab initio analysis”, *Scr. Mater.* **202**, 114000 (2021).
- [2] W. Chen, D. Dahliah, G.-M. Rignanese, and G. Hautier, “Origin of the low conversion efficiency in $\text{Cu}_2\text{ZnSnS}_4$ kesterite solar cells: the actual role of cation disorder”, *Energy Environ. Sci.*, - (2021).
- [3] M. Markov et al., “Ferroelectricity and multiferroicity in anti-Ruddlesden-Popper structures”, *Proc. Natl. Acad. Sci.* **118**, e2026020118 (2021).
- [4] A. Tal, W. Chen, and A. Pasquarello, “Vertex function compliant with the Ward identity for quasiparticle self-consistent calculations beyond GW ”, *Phys. Rev. B* **103**, L161104 (2021).
- [5] X. Gonze et al., “The ABINIT project: impact, environment and recent developments”, *Comput. Phys. Commun.* **248**, 107042 (2020).
- [6] T. Bischoff, J. Wiktor, W. Chen, and A. Pasquarello, “Nonempirical hybrid functionals for band gaps of inorganic metal-halide perovskites”, *Phys. Rev. Materials* **3**, 123802 (2019).
- [7] W. Chen, J. George, J. B. Varley, G.-M. Rignanese, and G. Hautier, “High-throughput computational discovery of $\text{In}_2\text{Mn}_2\text{O}_7$ as a high Curie temperature ferromagnetic semiconductor for spintronics”, *npj Comput. Mater.* **5**, 72 (2019).
- [8] S. Hadke, W. Chen, J. M. R. Tan, M. Guc, V. Izquierdo-Roca, G.-M. Rignanese, G. Hautier, and L. H. Wong, “Effect of Cd on cation redistribution and order-disorder transition in $\text{Cu}_2(\text{Zn}, \text{Cd})\text{SnS}_4$ ”, *J. Mater. Chem. A* **7**, 26927 (2019).
- [9] L. A. Burton, F. Ricci, W. Chen, G.-M. Rignanese, and G. Hautier, “High-throughput identification of electrides from all known inorganic materials”, *Chem. Mater.* **30**, 7521 (2018).
- [10] W. Chen, G. Miceli, G.-M. Rignanese, and A. Pasquarello, “Nonempirical dielectric-dependent hybrid functional with range separation for semiconductors and insulators”, *Phys. Rev. Materials* **2**, 073803 (2018).
- [11] W. Chen and A. Pasquarello, “Comment on ‘Fundamental resolution of difficulties in the theory of charged point defects in semiconductors’”, *Phys. Rev. Lett.* **120**, 039603 (2018).
- [12] Z. Guo, F. Ambrosio, W. Chen, P. Gono, and A. Pasquarello, “Alignment of redox levels at semiconductor–water interfaces”, *Chem. Mater.* **30**, 94 (2018).
- [13] G. Miceli, W. Chen, I. Reshetnyak, and A. Pasquarello, “Nonempirical hybrid functionals for band gaps and polaronic distortions in solids”, *Phys. Rev. B* **97**, 121112(R) (2018).
- [14] W. Chen and A. Pasquarello, “Accuracy of GW for calculating defect energy levels in solids”, *Phys. Rev. B* **96**, 020101(R) (2017).
- [15] A. Faghaninia et al., “A computational assessment of the electronic, thermoelectric, and defect properties of bournonite (CuPbSbS_3) and related substitutions”, *Phys. Chem. Chem. Phys.* **19**, 6743 (2017).
- [16] W. Chen, F. Ambrosio, G. Miceli, and A. Pasquarello, “*Ab initio* electronic structure of liquid water”, *Phys. Rev. Lett.* **117**, 186401 (2016).
- [17] W. Chen and A. Pasquarello, “Accurate band gaps of extended systems via efficient vertex corrections in GW ”, *Phys. Rev. B* **92**, 041115(R) (2015).
- [18] W. Chen and A. Pasquarello, “First-principles determination of defect energy levels through hybrid density functionals and GW ”, *J. Phys.: Condens. Matter* **27**, 133202 (2015).
- [19] W. Chen and A. Pasquarello, “Band-edge positions in GW : Effects of starting point and self-consistency”, *Phys. Rev. B* **90**, 165133 (2014).
- [20] K. Steiner, W. Chen, and A. Pasquarello, “Band offsets of lattice-matched semiconductor heterojunctions through hybrid functionals and G_0W_0 ”, *Phys. Rev. B* **89**, 205309 (2014).

- [21] W. Chen and A. Pasquarello, "Correspondence of defect energy levels in hybrid density functional theory and many-body perturbation theory", *Phys. Rev. B* **88**, 115104 (2013).
- [22] W. Chen and A. Pasquarello, "Band-edge levels in semiconductors and insulators: Hybrid density functional theory versus many-body perturbation theory", *Phys. Rev. B* **86**, 035134 (2012).
- [23] W. Chen, C. Tegenkamp, H. Pfnür, and T. Bredow, "Anomalous molecular orbital variation upon adsorption on a wide band gap insulator", *J. Chem. Phys.* **132**, 214706 (2010).
- [24] W. Chen, C. Tegenkamp, H. Pfnür, and T. Bredow, "Color centers in NaCl by hybrid functionals", *Phys. Rev. B* **82**, 104106 (2010).
- [25] W. Chen, C. Tegenkamp, H. Pfnür, and T. Bredow, "Insight from first-principles calculations into the interactions between hydroxybenzoic acids and alkali chloride surfaces", *J. Phys. Chem. C* **114**, 460 (2010).
- [26] W. Chen, C. Tegenkamp, H. Pfnür, and T. Bredow, "Tailoring band gaps of insulators by adsorption at surface defects: Benzoic acids on NaCl surfaces", *Phys. Rev. B* **79**, 235419 (2009).
- [27] W. Chen, C. Tegenkamp, H. Pfnür, and T. Bredow, "The interplay of van der Waals and weak chemical forces in the adsorption of salicylic acid on NaCl(001)", *Phys. Chem. Chem. Phys.* **11**, 9337 (2009).
- [28] M. Zhang, W. Chen, S.-J. Ding, Z.-Y. Liu, Y. Huang, Z.-W. Liao, and D. W. Zhang, "Physical and electrical characterization of atomic-layer-deposited Ru nanocrystals embedded into Al₂O₃ for memory applications", *J. Phys. D: Appl. Phys.* **41**, 032007 (2008).
- [29] W. Chen, W.-J. Liu, M. Zhang, S.-J. Ding, D. W. Zhang, and M.-F. Li, "Multistacked Al₂O₃-HfO₂-SiO₂ tunnel layer for high-density nonvolatile memory application", *Appl. Phys. Lett.* **91**, 022908 (2007).
- [30] W. Chen, Q.-Q. Sun, M. Xu, S.-J. Ding, D. W. Zhang, and L.-K. Wang, "Atomic layer deposition of hafnium oxide from tetrakis-(ethylmethylamino)-hafnium and water precursors", *J. Phys. Chem. C* **111**, 6495 (2007).
- [31] W. Chen, M. Zhang, D. Zhang, S.-J. Ding, J.-J. Tan, M. Xu, X.-P. Qu, and L.-K. Wang, "Growth of high-density Ru- and RuO₂-composite nanodots on atomic-layer-deposited Al₂O₃ film", *Appl. Surf. Sci.* **253**, 4045 (2007).
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- [33] H.-L. Lu, W. Chen, S.-J. Ding, D. W. Zhang, and L.-K. Wang, "DFT calculations of NH₃ adsorption and dissociation on gallium-rich GaAs(001)-4×2 surface", *Chem. Phys. Lett.* **445**, 188 (2007).
- [34] H.-L. Lu, M. Xu, S.-J. Ding, W. Chen, D. W. Zhang, and L.-K. Wang, "X-ray reflectometry and spectroscopic ellipsometry characterization of Al₂O₃ atomic layer deposition on HF-last and NH₃ plasma pretreatment Si substrates", *J. Mater. Res.* **22**, 1214 (2007).
- [35] Q.-Q. Sun, W. Chen, S.-J. Ding, M. Xu, H.-L. Lu, H.-C. Lindh-Rengifo, D. W. Zhang, and L.-K. Wang, "Comparative study of passivation mechanism of oxygen vacancy with fluorine in HfO₂ and HfSiO₄", *Appl. Phys. Lett.* **90**, 142904 (2007).
- [36] Q.-Q. Sun, W. Chen, S.-J. Ding, M. Xu, D. W. Zhang, and L.-K. Wang, "Effects of chlorine residue in atomic layer deposition hafnium oxide: A density-functional-theory study", *Appl. Phys. Lett.* **91**, 022901 (2007).
- [37] M. Zhang, W. Chen, S.-J. Ding, X.-P. Wang, D. W. Zhang, and L.-K. Wang, "Investigation of atomic-layer-deposited ruthenium nanocrystal growth on SiO₂ and Al₂O₃ films", *J. Vac. Sci. Technol., A* **25**, 775 (2007).
- [38] W. Chen, Q.-Q. Sun, S.-J. Ding, D. W. Zhang, and L.-K. Wang, "First principles calculations of oxygen vacancy passivation by fluorine in hafnium oxide", *Appl. Phys. Lett.* **89**, 152904 (2006).
- [39] S.-J. Ding, M. Zhang, W. Chen, D. W. Zhang, L.-K. Wang, X. P. Wang, C. Zhu, and M.-F. Li, "High density and program-erasable metal-insulator-silicon capacitor with a dielectric structure of SiO₂-HfO₂-Al₂O₃ nanolaminate-Al₂O₃", *Appl. Phys. Lett.* **88**, 042905 (2006).

- [40] H.-L. Lu, W. Chen, S.-J. Ding, M. Xu, D. W. Zhang, and L.-K. Wang, “Quantum chemical study of adsorption and dissociation of H_2S on the gallium-rich GaAs (001)- 4×2 surface”, *J. Phys. Chem. B* **110**, 9529 (2006).
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- [42] H.-L. Lu, M. Xu, S.-J. Ding, W. Chen, D. W. Zhang, and L.-K. Wang, “Quantum chemical study of the initial surface reactions of HfO_2 atomic layer deposition on the hydroxylated GaAs(001)- 4×2 surface”, *Appl. Phys. Lett.* **89**, 162905 (2006).
- [43] J. Ren, W. Chen, H. Lu, M. Xu, and W. Zhang, “Density functional theory study on surface reaction mechanism of atomic layer deposition of ZrO_2 on Si(100)- 2×1 ”, *Acta Chim. Sinica* **64**, 1133 (2006).
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- [45] M. Xu, C. Zhang, S.-J. Ding, H.-L. Lu, W. Chen, Q.-Q. Sun, D. W. Zhang, and L.-K. Wang, “Mechanism of interfacial layer suppression after performing surface $\text{Al}(\text{CH}_3)_3$ pretreatment during atomic layer deposition of Al_2O_3 ”, *J. Appl. Phys.* **100**, 106101 (2006).
- [46] W. Chen, H.-L. Lu, D. W. Zhang, M. Xu, J. Ren, J.-Y. Zhang, J.-T. Wang, and L.-K. Wang, “Density functional theory study of adsorption and dissociation of HfCl_4 and H_2O on Ge/Si(100)-(2×1): Initial stage of atomic layer deposition of HfO_2 on SiGe surface”, *Appl. Phys. Lett.* **86**, 142901 (2005).
- [47] W. Chen, D. W. Zhang, J. Ren, H.-L. Lu, J.-Y. Zhang, M. Xu, J.-T. Wang, and L.-K. Wang, “Density functional theory study of initial stage of ZrO_2 atomic layer deposition on Ge/Si(100)-(2×1) surface”, *Thin Solid Films* **479**, 73 (2005).
- [48] H.-L. Lu, W. Chen, S.-J. Ding, M. Xu, D. W. Zhang, and L.-K. Wang, “Initial surface reactions in atomic layer deposition of Al_2O_3 on the hydroxylated GaAs(001)- 4×2 surface”, *J. Phys.: Condens. Matter* **17**, 7517 (2005).

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