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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
• Many-body perturbation theory
• Nonempirical hybrid density functional
• High-throughput computational screening
• High-entropy alloys
• Thin-film solar cells
- 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

Good knowledge of FORTRAN, C, PYTHON, and GNU BASH.

Well versed in parallel computing (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

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-K 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.*

Selected Publications

- 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 \(2019\)](#).
- 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 \(2018\)](#).
- W. Chen and A. Pasquarello, “Accuracy of GW for calculating defect energy levels in solids”, [Phys. Rev. B 96, 020101\(R\) \(2017\)](#).
- W. Chen, F. Ambrosio, G. Miceli, and A. Pasquarello, “*Ab initio* electronic structure of liquid water”, [Phys. Rev. Lett. 117, 186401 \(2016\)](#).
- W. Chen and A. Pasquarello, “Accurate band gaps of extended systems via efficient vertex corrections in GW ”, [Phys. Rev. B 92, 041115\(R\) \(2015\)](#).

Publications in Chronological Order

- [1] X. Gonze et al., “The Abinit project: impact, environment and recent developments”, [Comput. Phys. Commun. 248, 107042 \(2020\)](#).
- [2] 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 \(2019\)](#).
- [3] 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 \(2019\)](#).
- [4] 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 \(2019\)](#).
- [5] 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 \(2018\)](#).
- [6] 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 \(2018\)](#).
- [7] 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 \(2018\)](#).
- [8] Z. Guo, F. Ambrosio, W. Chen, P. Gono, and A. Pasquarello, “Alignment of redox levels at semiconductor–water interfaces”, [Chem. Mater. 30, 94 \(2018\)](#).
- [9] 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\(R\) \(2018\)](#).
- [10] W. Chen and A. Pasquarello, “Accuracy of GW for calculating defect energy levels in solids”, [Phys. Rev. B 96, 020101\(R\) \(2017\)](#).
- [11] 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 \(2017\)](#).
- [12] W. Chen, F. Ambrosio, G. Miceli, and A. Pasquarello, “*Ab initio* electronic structure of liquid water”, [Phys. Rev. Lett. 117, 186401 \(2016\)](#).
- [13] W. Chen and A. Pasquarello, “Accurate band gaps of extended systems via efficient vertex corrections in GW ”, [Phys. Rev. B 92, 041115\(R\) \(2015\)](#).

- [14] 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).
- [15] W. Chen and A. Pasquarello, “Band-edge positions in *GW*: Effects of starting point and self-consistency”, *Phys. Rev. B* **90**, 165133 (2014).
- [16] 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).
- [17] 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).
- [18] 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).
- [19] 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).
- [20] W. Chen, C. Tegenkamp, H. Pfnür, and T. Bredow, “Color centers in NaCl by hybrid functionals”, *Phys. Rev. B* **82**, 104106 (2010).
- [21] 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).
- [22] 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).
- [23] 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).
- [24] W. Chen, W.-J. Liu, M. Zhang, S.-J. Ding, D. W. Zhang, and M.-F. Li, “Multistacked Al_2O_3 - HfO_2 - SiO_2 tunnel layer for high-density nonvolatile memory application”, *Appl. Phys. Lett.* **91**, 022908 (2007).
- [25] 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).
- [26] 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 RuO_2 -composite nanodots on atomic-layer-deposited Al_2O_3 film”, *Appl. Surf. Sci.* **253**, 4045 (2007).
- [27] S.-J. Ding, M. Zhang, W. Chen, D. W. Zhang, and L.-K. Wang, “Memory effect of metal-insulator-silicon capacitor with HfO_2 - Al_2O_3 multilayer and hafnium nitride gate”, *J. Electron. Mater.* **36**, 253 (2007).
- [28] H.-L. Lu, W. Chen, S.-J. Ding, D. W. Zhang, and L.-K. Wang, “DFT calculations of NH_3 adsorption and dissociation on gallium-rich $\text{GaAs}(001)\text{-}4\times 2$ surface”, *Chem. Phys. Lett.* **445**, 188 (2007).
- [29] 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 Al_2O_3 atomic layer deposition on HF-last and NH_3 plasma pretreatment Si substrates”, *J. Mater. Res.* **22**, 1214 (2007).
- [30] 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 HfO_2 and HfSiO_4 ”, *Appl. Phys. Lett.* **90**, 142904 (2007).
- [31] 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).
- [32] 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 SiO_2 and Al_2O_3 films”, *J. Vac. Sci. Technol., A* **25**, 775 (2007).
- [33] 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).

- [34] 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 $\text{SiO}_2\text{-HfO}_2\text{-Al}_2\text{O}_3$ nanolaminate- Al_2O_3 ”, *Appl. Phys. Lett.* **88**, 042905 (2006).
- [35] 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).
- [36] H.-L. Lu, W. Chen, S.-J. Ding, M. Xu, D. W. Zhang, and L.-K. Wang, “Quantum chemical study of the initial surface reactions in atomic layer deposition of TiN on the SiO_2 surface”, *J. Phys.: Condens. Matter* **18**, 5937 (2006).
- [37] 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).
- [38] 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).
- [39] J. Ren, H.-L. Lu, W. Chen, M. Xu, and D. W. Zhang, “Surface reaction mechanism of atomic layer deposition of HfO_2 on Ge(100)- 2×1 : A density functional theory study”, *Appl. Surf. Sci.* **252**, 8466 (2006).
- [40] 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).
- [41] 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).
- [42] 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).
- [43] 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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