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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, UC Louvain, Belgium
Institute of Condensed Matter and Nanosciences
Profs. Gian-Marco Rignanese and Geoffroy Hautier
• High-throughput computational screening of spin filters
• High-entropy alloys
• Thin-film solar cells (CZTS): disorder and its implications on the performance
- 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

04.2012 – 04.2016	Master's course: Computational Simulation and Physical Systems I & II Teaching assistance, EPFL
06.2013 – 04.2014	Supervising Master 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.*

Publications (chronological order)

- [1] 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 Computational Materials* **5**, 72 (2019).

- [2] L. A. Burton, F. Ricci, W. Chen, G.-M. Rignanese, and G. Hautier, “High-throughput identification of electrides from all known inorganic materials”, [Chemistry of Materials](#) **30**, 7521 (2018).
- [3] 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).
- [4] W. Chen and A. Pasquarello, “Comment on ‘Fundamental resolution of difficulties in the theory of charged point defects in semiconductors’”, [Physical Review Letter](#) **120**, 039603 (2018).
- [5] Z. Guo, F. Ambrosio, W. Chen, P. Gono, and A. Pasquarello, “Alignment of redox levels at semiconductor–water interfaces”, [Chemistry of Materials](#) **30**, 94 (2018).
- [6] G. Miceli, W. Chen, I. Reshetnyak, and A. Pasquarello, “Nonempirical hybrid functionals for band gaps and polaronic distortions in solids”, [Physical Review B](#) **97**, 121112(R) (2018).
- [7] W. Chen and A. Pasquarello, “Accuracy of *GW* for calculating defect energy levels in solids”, [Physical Review B](#) **96**, 020101(R) (2017).
- [8] A. Faghaninia, G. Yu, U. Aydemir, M. Wood, W. Chen, G.-M. Rignanese, G. J. Snyder, G. Hautier, and A. Jain, “A computational assessment of the electronic, thermoelectric, and defect properties of bournonite (CuPbSbS₃) and related substitutions”, [Physical Chemistry Chemical Physics](#) **19**, 6743 (2017).
- [9] W. Chen, F. Ambrosio, G. Miceli, and A. Pasquarello, “*Ab initio* electronic structure of liquid water”, [Physical Review Letters](#) **117**, 186401 (2016).
- [10] W. Chen and A. Pasquarello, “Accurate band gaps of extended systems via efficient vertex corrections in *GW*”, [Physical Review B](#) **92**, 041115(R) (2015).
- [11] W. Chen and A. Pasquarello, “First-principles determination of defect energy levels through hybrid density functionals and *GW*”, [Journal of Physics: Condensed Matter \(Invited Review\)](#) **27**, 133202 (2015).
- [12] W. Chen and A. Pasquarello, “Band-edge positions in *GW*: Effects of starting point and self-consistency”, [Physical Review B](#) **90**, 165133 (2014).
- [13] K. Steiner, W. Chen, and A. Pasquarello, “Band offsets of lattice-matched semiconductor heterojunctions through hybrid functionals and G_0W_0 ”, [Physical Review B](#) **89**, 205309 (2014).
- [14] W. Chen and A. Pasquarello, “Correspondence of defect energy levels in hybrid density functional theory and many-body perturbation theory”, [Physical Review B](#) **88**, 115104 (2013).
- [15] W. Chen and A. Pasquarello, “Band-edge levels in semiconductors and insulators: Hybrid density functional theory versus many-body perturbation theory”, [Physical Review B](#) **86**, 035134 (2012).
- [16] W. Chen, C. Tegenkamp, H. Pfnür, and T. Bredow, “Anomalous molecular orbital variation upon adsorption on a wide band gap insulator”, [Journal of Chemical Physics](#) **132**, 214706 (2010).
- [17] W. Chen, C. Tegenkamp, H. Pfnür, and T. Bredow, “Color centers in NaCl by hybrid functionals”, [Physical Review B](#) **82**, 104106 (2010).
- [18] W. Chen, C. Tegenkamp, H. Pfnür, and T. Bredow, “Insight from first-principles calculations into the interactions between hydroxybenzoic acids and alkali chloride surfaces”, [Journal of Physical Chemistry C](#) **114**, 460 (2010).
- [19] W. Chen, C. Tegenkamp, H. Pfnür, and T. Bredow, “Tailoring band gaps of insulators by adsorption at surface defects: Benzoic acids on NaCl surfaces”, [Physical Review B](#) **79**, 235419 (2009).
- [20] 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)”, [Physical Chemistry Chemical Physics](#) **11**, 9337 (2009).
- [21] 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”, [Applied Physics Letters](#) **91**, 022908 (2007).
- [22] 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”, [Journal of Physical Chemistry C](#) **111**, 6495 (2007).
- [23] 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”, [Applied Surface Science](#) **253**, 4045 (2007).

- [24] 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", *Journal of Electronic Materials* **36**, 253 (2007).
- [25] 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", *Chemical Physics Letters* **445**, 188 (2007).
- [26] 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", *Journal of Materials Research* **22**, 1214 (2007).
- [27] 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 ", *Applied Physics Letters* **90**, 142904 (2007).
- [28] 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", *Applied Physics Letters* **91**, 022901 (2007).
- [29] 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", *Journal of Vacuum Science & Technology A* **25**, 775 (2007).
- [30] 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", *Applied Physics Letters* **89**, 152904 (2006).
- [31] 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 SiO_2 - HfO_2 - Al_2O_3 nanolaminate- Al_2O_3 ", *Applied Physics Letters* **88**, 042905 (2006).
- [32] 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 $\text{GaAs}(001)\text{-}4\times 2$ surface", *Journal of Physical Chemistry B* **110**, 9529 (2006).
- [33] 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", *Journal of Physics: Condensed Matter* **18**, 5937 (2006).
- [34] 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 $\text{GaAs}(001)\text{-}4\times 2$ surface", *Applied Physics Letters* **89**, 162905 (2006).
- [35] 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 $\text{Si}(100)\text{-}2\times 1$ ", *Acta Chimica Sinica -Chinese Edition-* **64**, 1133 (2006).
- [36] J. Ren, H.-L. Lu, W. Chen, M. Xu, and D. W. Zhang, "Surface reaction mechanism of atomic layer deposition of HfO_2 on $\text{Ge}(100)\text{-}2\times 1$: A density functional theory study", *Applied Surface Science* **252**, 8466 (2006).
- [37] 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 ", *Journal of Applied Physics* **100**, 106101 (2006).
- [38] 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 $\text{Ge/Si}(100)\text{-(}2\times 1\text{)}$: Initial stage of atomic layer deposition of HfO_2 on SiGe surface", *Applied Physics Letters* **86**, 142901 (2005).
- [39] 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 $\text{Ge/Si}(100)\text{-(}2\times 1\text{)}$ surface", *Thin Solid Films* **479**, 73 (2005).
- [40] 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 $\text{GaAs}(001)\text{-}4\times 2$ surface", *Journal of Physics: Condensed Matter* **17**, 7517 (2005).