

## WEI CHEN

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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 ( <a href="https://github.com/wayn3/FNV">https://github.com/wayn3/FNV</a> )

## 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] 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).

- [2] 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 \(2018\)](#).
- [3] 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 \(2018\)](#).
- [4] Z. Guo, F. Ambrosio, W. Chen, P. Gono, and A. Pasquarello, “Alignment of redox levels at semiconductor–water interfaces”, [Chemistry of Materials \*\*30\*\*, 94 \(2018\)](#).
- [5] 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\(R\) \(2018\)](#).
- [6] W. Chen and A. Pasquarello, “Accuracy of *GW* for calculating defect energy levels in solids”, [Physical Review B \*\*96\*\*, 020101\(R\) \(2017\)](#).
- [7] 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 (CuPbSbS<sub>3</sub>) and related substitutions”, [Physical Chemistry Chemical Physics \*\*19\*\*, 6743 \(2017\)](#).
- [8] W. Chen, F. Ambrosio, G. Miceli, and A. Pasquarello, “*Ab initio* electronic structure of liquid water”, [Physical Review Letters \*\*117\*\*, 186401 \(2016\)](#).
- [9] W. Chen and A. Pasquarello, “Accurate band gaps of extended systems via efficient vertex corrections in *GW*”, [Physical Review B \*\*92\*\*, 041115\(R\) \(2015\)](#).
- [10] 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 \(2015\)](#).
- [11] W. Chen and A. Pasquarello, “Band-edge positions in *GW*: Effects of starting point and self-consistency”, [Physical Review B \*\*90\*\*, 165133 \(2014\)](#).
- [12] 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 \(2014\)](#).
- [13] 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 \(2013\)](#).
- [14] 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 \(2012\)](#).
- [15] 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 \(2010\)](#).
- [16] W. Chen, C. Tegenkamp, H. Pfnür, and T. Bredow, “Color centers in NaCl by hybrid functionals”, [Physical Review B \*\*82\*\*, 104106 \(2010\)](#).
- [17] 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 \(2010\)](#).
- [18] 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 \(2009\)](#).
- [19] 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 \(2009\)](#).
- [20] W. Chen, W.-J. Liu, M. Zhang, S.-J. Ding, D. W. Zhang, and M.-F. Li, “Multistacked Al<sub>2</sub>O<sub>3</sub>-HfO<sub>2</sub>-SiO<sub>2</sub> tunnel layer for high-density nonvolatile memory application”, [Applied Physics Letters \*\*91\*\*, 022908 \(2007\)](#).
- [21] 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 \(2007\)](#).
- [22] 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<sub>2</sub>-composite nanodots on atomic-layer-deposited Al<sub>2</sub>O<sub>3</sub> film”, [Applied Surface Science \*\*253\*\*, 4045 \(2007\)](#).
- [23] S.-J. Ding, M. Zhang, W. Chen, D. W. Zhang, and L.-K. Wang, “Memory effect of metal-insulator-silicon capacitor with HfO<sub>2</sub>-Al<sub>2</sub>O<sub>3</sub> multilayer and hafnium nitride gate”, [Journal of Electronic Materials \*\*36\*\*, 253 \(2007\)](#).

- [24] H.-L. Lu, W. Chen, S.-J. Ding, D. W. Zhang, and L.-K. Wang, "DFT calculations of  $\text{NH}_3$  adsorption and dissociation on gallium-rich  $\text{GaAs}(001)\text{-}4\times 2$  surface", *Chemical Physics Letters* **445**, 188 (2007).
- [25] 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  $\text{Al}_2\text{O}_3$  atomic layer deposition on HF-last and  $\text{NH}_3$  plasma pretreatment Si substrates", *Journal of Materials Research* **22**, 1214 (2007).
- [26] 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  $\text{HfO}_2$  and  $\text{HfSiO}_4$ ", *Applied Physics Letters* **90**, 142904 (2007).
- [27] 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).
- [28] 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  $\text{SiO}_2$  and  $\text{Al}_2\text{O}_3$  films", *Journal of Vacuum Science & Technology A* **25**, 775 (2007).
- [29] 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).
- [30] 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- $\text{Al}_2\text{O}_3$ ", *Applied Physics Letters* **88**, 042905 (2006).
- [31] 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  $\text{H}_2\text{S}$  on the gallium-rich  $\text{GaAs}(001)\text{-}4\times 2$  surface", *Journal of Physical Chemistry B* **110**, 9529 (2006).
- [32] 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  $\text{SiO}_2$  surface", *Journal of Physics: Condensed Matter* **18**, 5937 (2006).
- [33] 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  $\text{HfO}_2$  atomic layer deposition on the hydroxylated  $\text{GaAs}(001)\text{-}4\times 2$  surface", *Applied Physics Letters* **89**, 162905 (2006).
- [34] J. Ren, W. Chen, H. Lu, M. Xu, and W. Zhang, "Density functional theory study on surface reaction mechanism of atomic layer deposition of  $\text{ZrO}_2$  on  $\text{Si}(100)\text{-}2\times 1$ ", *Acta Chimica Sinica -Chinese Edition-* **64**, 1133 (2006).
- [35] J. Ren, H.-L. Lu, W. Chen, M. Xu, and D. W. Zhang, "Surface reaction mechanism of atomic layer deposition of  $\text{HfO}_2$  on  $\text{Ge}(100)\text{-}2\times 1$ : A density functional theory study", *Applied Surface Science* **252**, 8466 (2006).
- [36] 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  $\text{Al}_2\text{O}_3$ ", *Journal of Applied Physics* **100**, 106101 (2006).
- [37] 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  $\text{HfCl}_4$  and  $\text{H}_2\text{O}$  on  $\text{Ge/Si}(100)\text{-(}2\times 1\text{)}$ : Initial stage of atomic layer deposition of  $\text{HfO}_2$  on SiGe surface", *Applied Physics Letters* **86**, 142901 (2005).
- [38] 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  $\text{ZrO}_2$  atomic layer deposition on  $\text{Ge/Si}(100)\text{-(}2\times 1\text{)}$  surface", *Thin Solid Films* **479**, 73 (2005).
- [39] 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  $\text{Al}_2\text{O}_3$  on the hydroxylated  $\text{GaAs}(001)\text{-}4\times 2$  surface", *Journal of Physics: Condensed Matter* **17**, 7517 (2005).