Wei Chen
Nationality: Chinese
Date of Birth: 11 August 1980
Place of Birth: Shanghai, China
http://orcid.org/0000-0002-7496-0341
http://github.com/wayn3

Université Catholique de Louvain
Nanoscopic Physics Division (NAPS)
Chemin des Étoiles, 8 bte L7.03.01
B-1348, Louvain-la-Neuve, Belgium
wei.chen@uclouvain.be

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 Nanoscopic Physics Division (NAPS) (Profs. Gian-Marco Rignanese and Geoffroy Hautier) • Next-generation high-throughput computational screening of spin filters • High-entropy alloys • Thin-film solar cells (CZTS): disorder and its implications on the performance
04.2011 – 06.2016	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

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 and A. Pasquarello, "Comment on 'Fundamental resolution of difficulties in the theory of charged point defects in semiconductors'", Physical Review Letter **120**, 039603 (2018).

[2] 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).

[3] 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).

[4] W. Chen and A. Pasquarello, "Accuracy of *GW* for calculating defect energy levels in solids", Physical Review B **96**, 020101(R) (2017).

[5] 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).

[6] W. Chen, F. Ambrosio, G. Miceli, and A. Pasquarello, "*Ab initio* electronic structure of liquid water", Physical Review Letters **117**, 186401 (2016).

[7] W. Chen and A. Pasquarello, "Accurate band gaps of extended systems via efficient vertex corrections in *GW*", Physical Review B **92**, 041115(R) (2015).

[8] 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).

[9] W. Chen and A. Pasquarello, "Band-edge positions in *GW*: Effects of starting point and self-consistency", Physical Review B **90**, 165133 (2014).

[10] 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).

[11] 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).

[12] 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).

[13] 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).

[14] W. Chen, C. Tegenkamp, H. Pfnür, and T. Bredow, "Color centers in NaCl by hybrid functionals", Physical Review B **82**, 104106 (2010).

[15] 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).

[16] 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).

[17] 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).

[18] 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", Applied Physics Letters **91**, 022908 (2007).

[19] 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).

[20] 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", Applied Surface Science **253**, 4045 (2007).

[21] 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).

[22] 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 GaAs(001)-4×2 surface", Chemical Physics Letters **445**, 188 (2007).

[23] 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).

[24] 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).

[25] 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).

[26] 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).

[27] 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).

[28] 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).

[29] 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", Journal of Physical Chemistry B **110**, 9529 (2006).

[30] 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).

[31] 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", Applied Physics Letters **89**, 162905 (2006).

[32] 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 Chimica Sinica -Chinese Edition- **64**, 1133 (2006).

[33] 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", Applied Surface Science **252**, 8466 (2006).

[34] 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 $Al(CH_3)_3$ pretreatment during atomic layer deposition of Al_2O_3", Journal of Applied Physics **100**, 106101 (2006).

[35] 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", Applied Physics Letters **86**, 142901 (2005).

[36] 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).

[37] 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", Journal of Physics: Condensed Matter **17**, 7517 (2005).

Typeset by LaTeX. Updated on March 29, 2018.