Wei CHEN
Place of Birth: Shanghai, China
Present residence: Wavre, Belgium
https://orcid.org/0000-0002-7496-0341
https://github.com/wch3n

Université Catholique de Louvain
Institute of Condensed Matter and Nanosciences
Chemin des Étoiles, 8 bte L7.03.01
B-1348, Louvain-la-Neuve, Belgium
wei.chen_at_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, 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 $In_2Mn_2O_7$ 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 $In_2Mn_2O_7$ 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 $Cu_2(Zn,Cd)SnS_4$", 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 (CuPbSbS3) 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 GaAs(001)-4×2 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 SiO_2-HfO_2-Al_2O_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).

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[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 $Al(CH_3)_3$ pretreatment during atomic layer deposition of Al_2O_3", J. Appl. Phys. **100**, 106101 (2006).

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[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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