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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 · Multicomponent alloys · Emerging kesterite solar absorbers · Many-body perturbation theory · Nonempirical hybrid density functional · High-throughput computational screening
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

FORTRAN, C, PYTHON, GNU BASH, 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 – 06.2023	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	Masters thesis supervisor Project: Band-offset of lattice matched semiconductor heterojunctions (K. Steiner)

Recent Talks and Seminars

09.2021	E-MRS Fall Meeting 2021 Talk: "Origin of Low Conversion Efficiency of Cu_2ZnSnS_4 Kesterite Solar Absorber"
05.2021	MRS Spring Meeting 2021 Talk: "Origin of Low Conversion Efficiency of Cu_2ZnSnS_4 Kesterite Solar Absorber"
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"

Awards

05.2021	Best oral presentation, MRS Spring Meeting 2021

Miscellaneous

Referee for *Phys. Rev. Lett.*, *Phys. Rev. B*, *Appl. Phys. Lett.*, *J. Phys. Chem. Lett.*, *J. Phys. Chem.*, *npj Comput. Mater.*

Publications in Chronological Order

[1] W. Chen, A. Hilhorst, G. Bokas, S. Gorsse, P. J. Jacques, and G. Hautier, "A map of single-phase high-entropy alloys", Nat. Commun. **14**, 2856 (2023).

[2] W. Chen, S. M. Griffin, G.-M. Rignanese, and G. Hautier, "Nonunique fraction of Fock exchange for defects in two-dimensional materials", Phys. Rev. B **106**, L161107 (2022).

[3] S. P. Ramkumar, G. Petretto, W. Chen, H. P. C. Miranda, X. Gonze, and G.-M. Rignanese, "First-principles investigation of CZTS Raman spectra", Phys. Rev. Mater. **6**, 035403 (2022).

[4] D. M. Smiadak et al., "Quasi-1D electronic transport and isotropic phonon transport in the Zintl $Ca_5In_2Sb_6$", Mater. Today Phys. **22**, 100597 (2022).

[5] J. M. de Almeida, N. L. Nguyen, N. Colonna, W. Chen, C. Rodrigues Miranda, A. Pasquarello, and N. Marzari, "Electronic structure of water from koopmans-compliant functionals", J. Chem. Theory Comput. **17**, 3923 (2021).

[6] G. Bokas, W. Chen, A. Hilhorst, P. Jacques, S. Gorsse, and G. Hautier, "Unveiling the thermodynamic driving forces for high entropy alloys formation through big data ab initio analysis", Scr. Mater. **202**, 114000 (2021).

[7] W. Chen, D. Dahliah, G.-M. Rignanese, and G. Hautier, "Origin of the low conversion efficiency in Cu_2ZnSnS_4 kesterite solar cells: the actual role of cation disorder", Energy Environ. Sci. **14**, 3567 (2021).

[8] D. Evans, J. Chen, G. Bokas, W. Chen, G. Hautier, and W. Sun, "Visualizing temperature-dependent phase stability in high entropy alloys", npj Comput. Mater. **7**, 151 (2021).

[9] M. Markov et al., "Ferroelectricity and multiferroicity in anti–Ruddlesden–Popper structures", Proc. Natl. Acad. Sci. **118**, e2026020118 (2021).

[10] A. Tal, W. Chen, and A. Pasquarello, "Vertex function compliant with the Ward identity for quasiparticle self-consistent calculations beyond GW", Phys. Rev. B **103**, L161104 (2021).

[11] X. Gonze et al., "The ABINIT project: impact, environment and recent developments", Comput. Phys. Commun. **248**, 107042 (2020).

[12] 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).

[13] 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).

[14] 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).

[15] 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).

[16] 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).

[17] 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).

[18] Z. Guo, F. Ambrosio, W. Chen, P. Gono, and A. Pasquarello, "Alignment of redox levels at semiconductor–water interfaces", Chem. Mater. **30**, 94 (2018).

[19] 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).

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

[21] 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).

[22] W. Chen, F. Ambrosio, G. Miceli, and A. Pasquarello, "*Ab initio* electronic structure of liquid water", Phys. Rev. Lett. **117**, 186401 (2016).

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

[24] 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).

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

[26] 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).

[27] 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).

[28] 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).

[29] 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).

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

[31] 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).

[32] 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).

[33] 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).

[34] M. Zhang, W. Chen, S.-J. Ding, Z.-Y. Liu, Y. Huang, Z.-W. Liao, and D. W. Zhang, "Physical and electrical characterization of atomic-layer-deposited Ru nanocrystals embedded into Al2O3 for memory applications", J. Phys. D: Appl. Phys. **41**, 032007 (2008).

[35] 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).

[36] 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).

[37] 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).

[38] 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).

[39] 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).

[40] 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).

[41] 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).

[42] 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).

[43] 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).

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[46] 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).

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[50] 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).

[51] 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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[53] 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).

[54] 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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