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Nanoscopic Physics Division (NAPS)

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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 of 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”
- 04.2011 – 06.2016 Post-doctoral researcher, Ecole Polytechnique Fédérale de Lausanne (EPFL)
Chair of Atomic Scale Simulation
(Prof. Alfredo Pasquarello)
“Defects in solids through GW calculations”,
“*Ab initio* molecular dynamics of liquid water”

Coding skills

Good knowledge of FORTRAN, C, PYTHON, RUBY, 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

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. B*, *Appl. Phys. Lett.*

Publications (chronological order)

- [1] W. Chen, F. Ambrosio, G. Miceli, and A. Pasquarello, "Ab initio electronic structure of liquid water", *Physical Review Letters* **117**, 186401 (2016).
- [2] W. Chen, and A. Pasquarello, "Accurate band gaps of extended systems via efficient vertex corrections in GW", *Physical Review B (Rapid Comm.)* **92**, 041115(R) (2015).
- [3] 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).
- [4] W. Chen, and A. Pasquarello, "Band-edge positions in GW: Effects of starting point and self-consistency", *Physical Review B* **90**, 165133 (2014).
- [5] 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).

- [6] 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).
- [7] 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).
- [8] 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).
- [9] W. Chen, C. Tegenkamp, H. Pfnür, and T. Bredow, "Color centers in NaCl by hybrid functionals", *Physical Review B* **82**, 104106 (2010).
- [10] 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).
- [11] 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).
- [12] 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).
- [13] 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).
- [14] 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).
- [15] 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).
- [16] S.-J. Ding, M. Zhang, W. Chen, D. W. Zhang, and L.-K. Wang, "Memory effect of metal-insulator-silicon capacitor with HfO₂-Al₂O₃ multilayer and hafnium nitride gate", *Journal of Electronic Materials* **36**, 253 (2007).
- [17] H.-L. Lu, W. Chen, S.-J. Ding, D. W. Zhang, and L.-K. Wang, "DFT calculations of NH₃ adsorption and dissociation on gallium-rich GaAs(001)-4×2 surface", *Chemical Physics Letters* **445**, 188 (2007).
- [18] 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 Al₂O₃ atomic layer deposition on HF-last and NH₃ plasma pretreatment Si substrates", *Journal of Materials Research* **22**, 1214 (2007).
- [19] 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 HfO₂ and HfSiO₄", *Applied Physics Letters* **90**, 142904 (2007).
- [20] 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).
- [21] 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 SiO₂ and Al₂O₃ films", *Journal of Vacuum Science & Technology A* **25**, 775 (2007).
- [22] 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).
- [23] 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 SiO₂-HfO₂-Al₂O₃ nanolaminate-Al₂O₃", *Applied Physics Letters* **88**, 042905 (2006).
- [24] 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 H₂S on the gallium-rich GaAs (001)-4×2 surface", *Journal of Physical Chemistry B* **110**, 9529 (2006).
- [25] 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 SiO₂ surface", *Journal of Physics: Condensed Matter* **18**, 5937 (2006).

- [26] 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 HfO₂ atomic layer deposition on the hydroxylated GaAs(001)-4×2 surface", [Applied Physics Letters](#) **89**, 162905 (2006).
- [27] J. Ren, W. Chen, H. Lu, M. Xu, and W. Zhang, "Density functional theory study on surface reaction mechanism of atomic layer deposition of ZrO₂ on Si(100)-2×1", *Acta Chimica Sinica -Chinese Edition-* **64**, 1133 (2006).
- [28] J. Ren, H.-L. Lu, W. Chen, M. Xu, and D. W. Zhang, "Surface reaction mechanism of atomic layer deposition of HfO₂ on Ge(100)-2×1: A density functional theory study", [Applied Surface Science](#) **252**, 8466 (2006).
- [29] 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(CH₃)₃ pretreatment during atomic layer deposition of Al₂O₃", [Journal of Applied Physics](#) **100**, 106101 (2006).
- [30] 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 HfCl₄ and H₂O on Ge/Si(100)-(2×1): Initial stage of atomic layer deposition of HfO₂ on SiGe surface", [Applied Physics Letters](#) **86**, 142901 (2005).
- [31] 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 ZrO₂ atomic layer deposition on Ge/Si(100)-(2×1) surface", [Thin Solid Films](#) **479**, 73 (2005).
- [32] 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 Al₂O₃ on the hydroxylated GaAs(001)-4×2 surface", [Journal of Physics: Condensed Matter](#) **17**, 7517 (2005).

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