

## Curriculum Vitae

Department of Physics  
Faculty of Science, Kasetsart University  
Bangkok Thailand 10900

E-mail: p.reunchan@gmail.com  
fscippr@ku.ac.th  
Tel: (+66) 2-562-5555 #3532

### ***Educations***

Suranaree University of Technology, Thailand  
Ph.D. in Physics (theory of real materials), 2003–2009  
Advisor: Prof. Sukit Limpijumnong  
Dissertation topic “*First-principles study of selected defect complexes in semiconductors*”

Kasetsart University, Thailand  
B.Sc. Physics (Second Class Honors), 2000–2003

### ***Professional experiences***

- Lecturer in Physics, Faculty of Science, Kasetsart University, Thailand [ May 2012 – present]
- Postdoctoral Fellow, National Institute for Materials Science, Tsukuba, Japan [Nov 2010 – April 2012]
- Postdoctoral Fellow, Asia Pacific Center for Theoretical Physics, Pohang, Republic of Korea [Nov 2009 - Oct 2010]
- Research assistant, Materials department, University of California Santa Barbara, USA [Sep 2006 – Jun 2007]
- Research assistant, School of Physics, Suranaree University of Technology, Thailand [2004 – 2009]

### ***Research interests***

My current research interests cover:

- (1) Electronic properties of native defects and impurities in III-V and II-VI semiconductors.
- (2) Electronic structure and formation of complex defects in wide band gap semiconductors, including transparent conducting oxides (TCOs).
- (3) Hydrogen and diatomic molecules in semiconductors which have significant responsibility in electronic properties in semiconductors.
- (4) Defects and impurities in diluted nitrides and oxide alloys.
- (5) Hydrogen storage materials, i.e., hydrides and metal-dispersed nanomaterials
- (6) Doping and co-doping oxide materials for enhancing photocatalytic performance

### ***Honors and awards***

- Royal Golden Jubilee Ph.D. Program Full Scholarship, Thailand 2003–2009.
- Development and Promotion of Science and Technology Talents project (DPST) Full Scholarship, Thailand 2000–2003.
- Outstanding academic research, Suranaree University of Technology 18<sup>th</sup> anniversary 2008.
- Outstanding presentation (oral), The Royal Golden Jubilee Ph.D. Congress IX, 2008 Thailand. “CN molecule in GaAs: A first principles study”.
- Outstanding presentation (oral), The First National Symposium on Physics Graduate Research 2006 Thailand. “CN molecule in GaAs : A first principles study”.

### ***Research Grant Awarded***

- Preproposal Research Funds (PRF) from Faculty of Science, Kasetsart University, 2012-2013
- Research grant for supporting international publication from Kasetsart University Research and Development Institute, 2013 : “Nitrogen doping in strontium titanate for enhancing photocatalytic activities under visible-light irradiation: theory and computations”
- Research Fund for DPST Graduate with First Placement, 2013-2015: “Energy band gap engineering of perovskite oxides for photocatalytic hydrogen production from visible light: Theory and computations”

### ***Research experiences***

My research experiences cover the studies of defects, impurities and complexes in wide band-gap semiconductors as well as nanomaterials for hydrogen storage. The first-principles calculations based on density functional theory (DFT) using plane-wave basis set, pseudopotential with LDA, GGA-PBE or HSE functionals are used in my research.

### ***Postdoctoral Fellows***

**National Institute for Materials Science**, Tsukuba, Japan, Nov 2010-April 2012

*supervisor*: Dr. Naoto Umezawa

- Cr-doped SrTiO<sub>3</sub> photocatalyst and codoping for photocatalytic enhancement based on DFT
- Native defects and hydrogen in Ag<sub>3</sub>PO<sub>4</sub>

**Asia Pacific Center for Theoretical Physics**, Pohang, South Korea, Nov 2009–Oct 2010

*supervisor*: Dr. Xin Zhou

- Definition of H-bonds in liquid water using trajectory mapping method

*supervisor*: Prof. Seung-Hoon Jhi

- Hydrogen storage materials focusing on incorporation of metal atoms onto nanostructures

### ***Visiting research assistant***

**Materials department, University of California Santa Barbara**, USA, Sep 2006–June 2007.

*supervisor*: Prof. Chris G. Van de Walle     *co-supervisor*: Dr. Anderson Janotti

- The mechanism of mutual passivation between group-IV (Si and Ge) and N in GaAsN alloys
- Native defects and impurities in In<sub>2</sub>O<sub>3</sub> (transparent conducting oxide)

### ***Research assistant***

**School of Physics, Suranaree University of Technology**, Thailand, 2003–2009.

*supervisor*: Prof. Sukit Limpijumnong

- Native point defects and impurities in *wurtzite* aluminum nitride (AlN).
- Native defects donor in ZnO, study their complex with N, expecting to be a leading donor.
- CN molecule in GaAs and GaP, investigating their favorable site and vibration frequencies.
- Frenkel pairs in GaN, investigates their electronic structure, migration and recombination barrier.
- Basic studies of TiO<sub>2</sub>, PbTiO<sub>3</sub> properties and surface reconstruction in Si(100).

### ***Skills***

- First-principles calculation codes i.e. VASP (Vienna ab-initio simulation package) and CPMD (Car-Parrinello Molecular Dynamics code)
- Data and crystal virtualizing programs such as OpenDX, Xcrysden, VESTA, Rasmol, Crystal maker

- Computer hardware installation / assemble, trouble shooting and basic designing for high performance computing clusters.
- Linux operating system installation and some applications, e.g., Xmgrace.
- Windows operating system installation and common applications
- Basic scripting, e.g., bash script, Python

### ***Activities***

- Participated in conducting the workshop on band structure/supercell calculations at University Sains Malaysia, November 24-26, 2013, Penang, Malaysia
- Chaired a condensed matter physics session in Siam Physics Congress 2013, Thailand
- Chaired a session for symposium Q in International Conference on Materials for Advanced Technologies 2009, Singapore
- Visited Asia Pacific Center for Theoretical Physics (APCTP) June 7–16, 2009 POSTECH, Pohang, South Korea.
- Attended the 2<sup>nd</sup> AOFSRR summer school “Cheiron School 2008” September 29–October 8 2008 Spring-8, Hyogo, Japan.
- Attended summer school “Quantum Monte Carlo from Minerals and Materials to Molecule” July 9 – 19, 2007 University of Illinois at Urbana-Champaign, IL USA.

### ***Presentations***

- Siam Physics Congress 2014, Nakhon ratchasima, Thailand. “Theoretical Design of Highly Active SrTiO<sub>3</sub>-based Photocatalyst from Doping Scheme toward Solar Energy Utilization for Hydrogen Production” (Oral, invited)
- Siam Physics Congress 2013, Chiangmai, Thailand. “Metal-dispersed porous graphene for hydrogen storage” (Poster).
- Asian Consortium Conference on Computational Materials Science – Work group meeting on Computational Design of Materials for Energy Conversion and Storage, Taiwan. “Theoretical Design of Highly Active SrTiO<sub>3</sub>-based Photocatalyst from Doping Scheme toward Solar Energy Utilization for Hydrogen Production” (Oral, invited).
- The 14<sup>th</sup> Asian Workshop on First-Principles Electronic Structure Calculations 2011, Japan. “Theory of Chromium-doped SrTiO<sub>3</sub> photocatalyst” (Poster).
- IUMRS-ICA 2011, 12<sup>th</sup> international conference in Asia 2011, Taiwan. “Theoretical study of Chromium-doped SrTiO<sub>3</sub> photocatalyst” (Poster).
- The 13<sup>th</sup> Asian Workshop on First-Principles Electronic Structure Calculations 2010, Korea. “Role of metals on porous graphene for hydrogen storage” (Poster)
- The 7<sup>th</sup> Asian Meeting on Ferroelectricity and 7<sup>th</sup> Asian meeting on Electroceramics 2010, Jeju, Korea. “Vacancy defects in In<sub>2</sub>O<sub>3</sub>: A first-principles study” (Oral)
- The 5<sup>th</sup> Asian Consortium Conference on Computational Materials Science 2009, Vietnam. “Silicon and Carbon impurities in GaAs<sub>1-x</sub>N<sub>x</sub>” (Oral)
- International Conference on Materials for Advanced Technologies 2009, Singapore. “First-principles study of Gallium-Frenkel pairs in GaN” (Oral)
- JRG seminar 2009, APCTP, Korea. “Diatomic Molecules in Dilute Nitrides: A First-Principles Study” (Oral)
- The Siam Physics Congress 2009, Thailand. “Vacancy Defects in In<sub>2</sub>O<sub>3</sub>” (Poster)
- The 34<sup>th</sup> Congress in Science and Technology Thailand. “CN molecule in GaAs” (Oral)

- The Royal Golden Jubilee Ph.D. Congress IX, 2008 Thailand. “CN molecule in GaAs : A first principles study” (Oral)
- The Siam Physics Congress 2008, Thailand “Mutual passivation of electrically active and isovalent impurities in GaAsN alloys” (Oral)
- The First National Symposium on Physics Graduate Research 2006, Thailand. “ CN molecule in GaAs : A first principles study” (Oral)
- The 5<sup>th</sup> National School on Photoemission, National Synchrotron Research Center, Nakhon-ratchasima, Thailand: May 2006 “CN molecule in GaAs : A first principles study” (Oral)

***Publications (refereed journals with journal impact factors)***

1. Pakpoom Reunchan, Naoto Umezawa  
Native defects and hydrogen impurities in Ag<sub>3</sub>PO<sub>4</sub>  
Physical Review B **87**, 245205 (2013).
2. Hua Xu, Pakpoom Reunchan, Shuxin Ouyang, Hua Tong, Naoto Umezawa, Tetsuya Kako, Yuangjian Zhang, Jinhua Ye  
Anatase TiO<sub>2</sub> Single Crystals Exposed with High-Reactive {111} Facets Towards Efficient H<sub>2</sub> Evolution  
Chemistry of Materials **25**, 405 (2013).
3. Pakpoom Reunchan, Shuxin Ouyang, Naoto Umezawa, Hua Xu, Yuangjian Zhang, Jinhua Ye  
Theoretical design of highly active SrTiO<sub>3</sub>-based photocatalysts by a codoping scheme towards solar energy utilization for hydrogen production  
Journal of Materials Chemistry A **1**, 4221 (2013).
4. Sirichok Jungthawan, Pakpoom Reunchan, Sukit Limpijumnong  
Theoretical study of strained porous graphene structures and their gas separation properties  
Carbon **54**, 359 (2013).
5. Pakpoom Reunchan, Naoto Umezawa, Shuxin Ouyang, Jinhua Ye  
Mechanism of photocatalytic activities in Cr-doped SrTiO<sub>3</sub> under visible-light irradiation: an insight from hybrid density-functional calculations  
Phys. Chem. Chem. Phys. **14**, 1876 (2012).
6. Kui Xie, Naoto Umezawa, Ning Zhang, Pakpoom Reunchan, Yuanjian Zhang, Jinhua Ye  
Self-doped SrTiO<sub>3-δ</sub> photocatalyst with enhanced activity for artificial photosynthesis under visible light  
Energy Environ. Sci. **4**, 4211 (2011).
7. Pakpoom Reunchan, Xin Zhou, Sukit Limpijumnong, Anderson Janotti, Chris G. Van de Walle  
Vacancy defects in indium oxide: An *ab-initio* study  
Curr. Appl. Phys. **11**, S296 (2011).
8. Pakpoom Reunchan and Seung-Hoon Jhi  
Metal-dispersed porous graphene for hydrogen storage  
Appl. Phys. Lett. **98**, 093103 (2011).
9. Sukit Limpijumnong, Pakpoom Reunchan, Anderson Janotti, Chris G. Van de Walle  
Hydrogen doping in indium oxide: An *ab-initio* study  
Phys. Rev. B **80**, 193202 (2009).

10. Sukit Limpijumnong, Pakpoom Reunchan, Anderson Janotti, Chris G. Van de Walle  
Carbon-nitrogen molecules in GaAs and GaP  
Phys. Rev. B **77**, 195209 (2008).
11. A. Janotti, P. Reunchan, S. Limpijumnong, C. G. Van de Walle  
Mutual passivation of electrically active and isovalent impurities in dilute nitrides.  
Phys. Rev. Lett. **100**, 045505 (2008).
12. D.C. Look, G.C. Farlow, Pakpoom Reunchan, Sukit Limpijumnong, S.B. Zhang, K. Nordlund  
Evidence for native-defect donors in *n*-type ZnO  
Phys. Rev. Lett. **95**, 225502 (2005).

## *References*

Prof. Dr. Sukit Limpijumnong  
Suranaree University of Technology (SUT),  
Nakhon-Ratchasima, Thailand 30000  
Phone: (+66) 8-1120-3830  
E-mail: [sukit@sut.ac.th](mailto:sukit@sut.ac.th), [konesarn@gmail.com](mailto:konesarn@gmail.com)  
<http://110.164.94.173/ccmp/sukit/>

Dr. Anderson Janotti  
Materials Department, University of California,  
Santa Barbara (UCSB), CA 93106-5050  
Phone: (+1) 805-893-7499  
Fax: (+1) 805-893-5029  
Email: [ajanotti@mrl.ucsb.edu](mailto:ajanotti@mrl.ucsb.edu), [janotti@engineering.ucsb.edu](mailto:janotti@engineering.ucsb.edu)  
<http://research.mrl.ucsb.edu/~vdwgroup/ajanotti/>

Prof. Dr. Chris G. Van de Walle  
Materials Department, University of California,  
Santa Barbara (UCSB), CA 93106-5050  
Phone: (+1) 805-893-7144  
Fax: (+1) 805-893-8983  
E-mail: [vandewalle@mrl.ucsb.edu](mailto:vandewalle@mrl.ucsb.edu)  
<http://www.mrl.ucsb.edu/~vandewalle/>

Prof. Dr. Seung-Hoon Jhi  
Department of Physics, Pohang University of Science and  
Technology (POSTECH), Pohang, South Korea 790-784  
Phone: (+82) 54-279-5921  
E-mail: [jhish@postech.ac.kr](mailto:jhish@postech.ac.kr)  
<http://cnpl.postech.ac.kr/>

Dr. Naoto Umezawa  
National Institute for Materials Science,  
Tsukuba, Ibaraki, Japan 305-0047  
Phone: (+81) 29-860-4547  
E-mail: [UMEZAWA.naoto@nims.go.jp](mailto:UMEZAWA.naoto@nims.go.jp)