

# Curriculum Vitae

Naoto Umezawa

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## **Education**

2000-2003 Ph.D, Department of Physics, University of Tokyo

1998-2000 Degree of Master, Department of Condensed Matter Physics, Tokyo Institute of Technology

1993-1998 Degree of Bachelor, Faculty of Physics, Aoyama Gakuin University

## **Professional Experience**

2008-present Senior researcher, National Institute for Materials Science, Japan

2014-present Guest associate professor, Hokkaido University, Japan

2013 Research visitor, Aarhus University, Denmark

2011-present Guest professor, Tianjin University, China

2006-2007 Research visitor, University of California, Santa Barbara

2006-2008 Researcher, National Institute for Materials Science, Japan

2004-2006 Postdoctoral Scientist, National Institute for Materials Science, Japan

2003-2004 Postdoctoral Scientist, University of Southern California

## **Honors**

- JJAP Excellent Paper Award, 2007
- Award for Encouragement of Research of Materials Science of Materials Research Society of Japan, 2005

## **Research Interests**

- Theoretical design of inorganic materials using first-principles calculations
- Defects and impurities in insulators and semiconductors
- Electronic structures of oxide materials applied to photocatalysts, photovoltaics, or opto-electronics.
- Chemical reactions on surfaces of catalysts
- Methodology development of highly accurate first-principles electronic structure calculations

## **Professional Activities**

### **Member:**

APS (American Physical Society)

### **Referee/Reviewer:**

**Journals:** Physical Review Letters, Journal of Applied Physics, Applied Physics Express, Applied Physics Letters, IEEE Electron Device Letters, Japan Journal of Applied Physics, Advanced Functional Materials, Physical Chemistry Chemical Physics, Applied Surface Science, ChemPhysChem, The Journal of Chemical

Physics, Surface Science, Journal of Electronic Materials, APL Materials, MRS Proceedings, Physical Review B, ACS Applied Materials & Interfaces, CrystEngComm, The Journal of Physical Chemistry, Computational Materials Science, Journal of Materials Chemistry A, Physical Review Applied

### **Contracts and Grants:**

Japan Society for the Promotion of Science (JSPS), Japan Science and Technology Agency (JST), Saint-Gobain, LG

### **Funding records**

- 2009-2010 0.50mil. JPY (\$4,000), “Transparent electric conductor”, Saint-Gobain
- 2009-2010 4.55 mil. JPY (\$37,000), “Property control of oxides from impurity doping toward materials design”, JSPS Grant-in-Aid for Young Scientists (B)
- 2010-2013 38.53 mil. JPY (\$318,000), “Development of high performance photocatalysts from ubiquitous elements”, JST Precursory Research for Embryonic Science and Technology (PRESTO)
- 2013-2013 1.39 mil. JPY (\$11,000), “Theoretical study of the role of co-catalysts in photocatalysis reactions”, JSPS Researcher Exchange Program (Denmark)
- 2010-2015 50.00 mil. JPY (\$413,000), “Research and development of Innovative Materials for Environmental Remediation”, NIMS project
- 2013-2015 12.80 mil. JPY (\$99,000), “Theoretical study of photocatalytic activities on graphene-like material/TiO<sub>2</sub> interfaces”, JSPS postdoctoral fellowship (acting as a host)
- 2013-2015 6.00 mil JPY (\$49,000), “Development of plasmonics materials using ceramics metals ”, JST Core Research for Evolutional Science and Technology (CREST)
- 2014-2015 0.50mil. JPY (\$4,000), “Development of novel photocatalysts for organic degradation”, LG

### **Publications**

- (74) Junjie Wang, **Naoto Umezawa\***, and Hideo Hosono, “Mixed Valence Tin Oxides as Novel van der Waals Materials: Theoretical Predictions and Potential Applications” *Adv. Energy Mater.* 2015, DOI: 10.1002/aenm.201501190.
- (73) Shunsuke Yagi, Ikuya Yamada, Hirofumi Tsukasaki, Akihiro Seno, Makoto Murakami, Hiroshi Fujii, Hungru Chen, **Naoto Umezawa**, Hideki Abe, Norimasa Nishiyama and Shigeo Mori, “Covalency-reinforced oxygen evolution reaction catalyst” *Nat. Commun.*, 2015, DOI: 10.1038/ncomms9249.
- (72) Akira Yoko, Makoto Akizuki, Naohisa Hirao, Shinji Kohara, Mukesh Kumar, **Naoto Umezawa**, Takahisa Ohno, Yoshito Oshima, “In situ synchrotron high-energy X-ray diffraction for elucidation of millisecond-order dynamics of the formation of barium zirconate nanoparticles in supercritical water” *J. Supercritical Fluids*, [doi:10.1016/j.supflu.2015.08.002](https://doi.org/10.1016/j.supflu.2015.08.002)
- (71) Hungru Chen, James A. Dawson, and **Naoto Umezawa\***, “Anisotropic nature of anatase TiO<sub>2</sub> and its (001) surface electronic states” *Phys. Rev. Appl.* **4**, 014007, 2015.
- (70) Peng Li, Wei Zhou, Xin Wang, Yan Zhang, **Naoto Umezawa\***, Hideki Abe\*, Jinhua Ye, and Defa Wang, “Effects of cation concentration on photocatalytic performance over magnesium vanadates” *Appl. Phys. Lett. Mater.* **3**, 104405, 2015.
- (69) Wenqiang Dang, Hungru Chen, **Naoto Umezawa\***, and Junying Zhang\*, ”Electronic Structures of

- Anatase (TiO<sub>2</sub>)<sub>1-x</sub>(TaON)<sub>x</sub> Solid Solutions: First-Principles Study” *Phys. Chem. Chem. Phys.*, **17**, 17980-17988, 2015.
- (68) Wei Zhou and **Naoto Umezawa\***, “Band gap engineering of bulk and nanosheet SnO: and insight into the interlayer Sn-Sn lone pair interactions” *Phys. Chem. Chem. Phys.*, **17**, 17816-17820, 2015.
- (67) Peng Li, **Naoto Umezawa\***, Hideki Abe\*, and Jinhua Ye, “Novel visible-light sensitive vanadate 1 photocatalysts for water oxidation: implications from density functional theory calculations”, *J. Mater. Chem. A* **3**, 10720-10723, 2015.
- (66) Rajesh Kodiyath, Gubbala V. Ramesh, Eva Koudelkova, Toyokazu Tanabe, Mikio Ito, Maidhily Manikandan, Shigenori Ueda, Takeshi Fujita, **Naoto Umezawa**, Hidenori Noguchi, Katsuhiko Arigad and Hideki Abe, “Promoted C–C bond cleavage over intermetallic 1 TaPt<sub>3</sub> catalyst toward low-temperature energy extraction from ethanol”, *Energy & Environmental Science* **8**, 1685-1689, 2015.
- (65) Hungru Chen and **Naoto Umezawa**, “Artificial layered perovskite oxides A(B<sub>0.5</sub>B'<sub>0.5</sub>)O<sub>3</sub> as potential solar energy conversion materials”, *J. Appl. Phys.* **117**, 055106 (1-5), 2015.
- (64) Pakpoom Reunchan and **Naoto Umezawa**, “Sulfur and Silicon Doping in Ag<sub>3</sub>PO<sub>4</sub>”, *J. Phys. Chem. C*, **119**, 2284-2289, 2015.
- (63) Mukesh Kumar, **Naoto Umezawa**, and Motoharu Imai, “Structural, electronic and optical characteristics of SrGe<sub>2</sub> and BaGe<sub>2</sub>: A combined experimental and computational study”, *J. Alloys and Compounds* **630**, 126-132, 2015.
- (62) Mohamed B. Zakaria, Ming Hu, Masataka Imura, Rahul R. Salunkhe, **Naoto Umezawa**, Hicham Hamoudi, Alexei A. Belik, and Yusuke Yamauchi, “Single-Crystal-like Nanoporous Spinel Oxides: A Strategy for Synthesis of Nanoporous Metal Oxides Utilizing Metal-Cyanide Hybrid Coordination Polymers”, *Chemistry A European Journal*, **20**, 17375-17384, 2014.
- (61) Jian Ren, Shuxin Ouyang, Hungru Chen, **Naoto Umezawa**, Da Lu, Defa Wang, Hua Xu, Jinhua Ye, “Effective Mineralization of Organic Dye under Visible-Light Irradiation over Electronic-Structure-Modulated Sn(Nb<sub>1-x</sub>Ta<sub>x</sub>)<sub>2</sub>O<sub>6</sub> Solid Solutions”, *Applied Catalysis B: Environmental*, **168-169**, 243-249, 2015.
- (60) Ming Zhao, Hua Xu, Hungru Chen, Shuxin Ouyang, **Naoto Umezawa**, Defa Wang, Jinhua Ye, “Photocatalytic reactivity of {121} and {211} facets of brookite TiO<sub>2</sub> crystals”, *J. Mater. Chem. A*, **3**, 2331-2337, 2015.
- (59) Hideki Abe, Hideki Yoshikawa, **Naoto Umezawa**, Ya Xu, Govindachetty Saravanan, Gubbala V. Ramesh, Toyokazu Tanabe, Rajesh Kodiyath, Shigenori Ueda, Nobuaki Sekido, Yoko Yamabe-Mitarai, Masahiko Shimoda, Takahisa Ohno, Futoshi Matsumot and Takayuki Komatsu, “Correlation between the Surface Electronic Structure and CO-oxidation Activity of Pt Alloys”, *Phys. Chem. Chem. Phys.*, **17**, 4879-4887, 2015.
- (58) Gubbala V. Ramesh, Rajesh Kodiyath, Toyokazu Tanabe, Maidhily Manikandan, Takeshi Fujita, **Naoto Umezawa**, Shigenori Ueda, Shinsuke Ishihara, Katsuhiko Ariga, and Hideki Abe, “Stimulation of Electro-oxidation Catalysis by Bulk-Structural Transformation in Intermetallic ZrPt<sub>3</sub> Nanoparticles”, *ACS Applied Materials & Interfaces*, **6**, 16124-16130, 2014.
- (57) Hungru Chen and **Naoto Umezawa**, “Sensitization of Perovskite Strontium Stannate SrSnO<sub>3</sub> towards Visible-Light Absorption by Doping” *International Journal of Photoenergy*, <http://dx.doi.org/10.1155/2014/643532>
- (56) Hungru Chen and **Naoto Umezawa**, “Effect of cation arrangement on the electronic structures of the

- perovskite solid solutions  $(\text{SrTiO}_3)_{1-x}(\text{LaCrO}_3)_x$  from first principles” *Phys. Rev. B* **90** (4), 045119 (1-7), 2014.
- (55) Hungru Chen and **Naoto Umezawa**, “Hole localization, migration, and the formation of peroxide anion in perovskite  $\text{SrTiO}_3$ ”, *Phys. Rev. B* **90** (3), 035202 (1-5), 2014.
- (54) Mukesh Kumar, **Naoto Umezawa**, and Motoharu Imai, “ $\text{BaSi}_2$  as a promising low-cost, earth-abundant material with large optical activity for thin-film solar cells: a hybrid density functional study” *Applied Physics Express* **7**, 071203, 2014.
- (53) Mukesh Kumar, **Naoto Umezawa**, and Motoharu Imai, “ $(\text{Sr,Ba})(\text{Si,Ge})_2$  for thin-film solar-cell applications: First-principles study” *J. Appl. Phys.* **115**, 203718, 2014.
- (52) Hua Xu, Shuxin Ouyang, Lequan Liu, Pakpoom Reunchan, **Naoto Umezawa** and Jinhua Ye, “Recent advances in  $\text{TiO}_2$ -based photocatalysis” *J. Mater. Chem. A*, **2**, 12642-12661, 2014.
- (51) Lequan Liu, Peng Li, Boonchun Adisak, Shuxin Ouyang, **Naoto Umezawa**, Jinhua Ye, Rajesh Kodiyath, Toyokazu Tanabe, Gubbala V. Ramesh, Shigenori Ueda and Hideki Abe, “Gold photosensitized  $\text{SrTiO}_3$  for visible-light water oxidation induced by Au interband transitions”, *J. Mater. Chem. A*, **2**, 9875-9882, 2014.
- (50) Francis Malar Auxilia, Shinsuke Ishihara, Saikat Mandal, Toyokazu Tanabe, Govindachetty Saravanan, Gubbala V. Ramesh, **Naoto Umezawa**, Toru Hara, Ya Xu, Shunichi Hishita, Yusuke Yamauchi, Arivuoli Dakshanamoorthy, Jonathan P. Hill, Katsuhiko Ariga, and Hideki Abe, “Low-Temperature Remediation of NO Catalyzed by Interleaved  $\text{CuO}$  Nanoplates” *Adv. Mater.* **26**, 4481-4485, 2014.
- (49) Peng Li, Hua Xu, Lequan Liu, Tetsuya Kako, **Naoto Umezawa**, Hideki Abe, and Jinhua Ye, “Constructing cubic-orthorhombic surface-phase junctions of  $\text{NaNbO}_3$  towards significant enhancement of  $\text{CO}_2$  photoreduction” *J. Mater. Chem. A*, **2**, 5606-5609, 2014.
- (48) Maidhily Manikandan, Toyokazu Tanabe, Peng Li, Shigenori Ueda, Gubbala V. Ramesh, Rajesh Kodiyath, Junjie Wang, Toru Hara, Arivuoli Dakshanamoorthy, Shinsuke Ishihara, Katsuhiko Ariga, Jinhua Ye, **Naoto Umezawa**, and Hideki Abe, “Photocatalytic Water Splitting under Visible Light by Mixed-Valence  $\text{Sn}_3\text{O}_4$ ” *ACS Applied Materials & Interfaces*, **6**, 3790-3793, 2014.
- (47) David James Martin, **Naoto Umezawa**, Xiaowei Chen, Jinhua Ye, and Junwang Tang, “Facet engineered  $\text{Ag}_3\text{PO}_4$  for efficient water photooxidation” *Energy & Environmental Sci.* **6**, 3380-3386, 2013.
- (46) Pakpoom Reunchan and **Naoto Umezawa**, “Native defects and hydrogen impurities in  $\text{Ag}_3\text{PO}_4$ ” *Phys. Rev. B* **87** (24), 245205 (1-5), 2013.
- (45) Adisak Boonchun, **Naoto Umezawa**, Takahisa Ohno, Shuxin Ouyang, and Jinhua Ye, “Role of photoexcited electrons in hydrogen evolution from platinum co-catalysts loaded on anatase  $\text{TiO}_2$ : First-principles study” *J. Mater. Chem. A*, **1**, 6664-6669, 2013.
- (44) Pakpoom Reunchan, Shuxin Ouyang, **Naoto Umezawa**, Hua Xu, Yuanjian Zhang, and Jinhua Ye, “Theoretical design of highly active  $\text{SrTiO}_3$ -based photocatalysts by a codoping scheme towards solar energy utilization for hydrogen production” *J. Mater. Chem. A*, **1**, 4221-4227, 2013
- (43) Hua Xu, Pakpoom Reunchan, Shuxin Ouyang, Hua Tong, **Naoto Umezawa**, Tetsuya Kako, and Jinhua Ye, “Anatase  $\text{TiO}_2$  single crystals exposed with high-reactive  $\{111\}$  facets toward efficient  $\text{H}_2$  evolution” *Chemistry of Materials*, **25**, 405-411, 2013.
- (42) Tetsuya Kako, **Naoto Umezawa**, Kui Xie, and Jinhua Ye, “Undoped visible-light-sensitive titania photocatalyst” *J. Mater. Sci.* **48**, 108 (2013).
- (41) **Naoto Umezawa** and Jinhua Ye, “Role of complex defects in photocatalytic activities of nitrogen-doped

- anatase TiO<sub>2</sub>”, *Phys. Chem. Chem. Phys.*, **14**, 5924-5934, 2012.
- (40) Shuxin Ouyang, Hua Tong, **Naoto Umezawa**, Junyu Cao, Peng Li, Yingpu Bi, Yuanjian Zhang, and Jinhua Ye, “Surface-Alkalinization-Induced Enhancement of Photocatalytic H<sub>2</sub> Evolution over SrTiO<sub>3</sub>-Based Photocatalysts”, *J. Am. Chem. Soc.* **134**, 1974-1977, 2012.
- (39) **Naoto Umezawa** and Kenji Shiraishi, “Theoretical model for artificial structure modulation of HfO<sub>2</sub>/SiO<sub>x</sub>/Si interface by deposition of a dopant material”, *Appl. Phys. Lett.* **100** (9), 092904 (1-4), 2012.
- (38) Pakpoom Reunchan, **Naoto Umezawa**, Shuxin Ouyang, and 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**, 1876-1880, 2012.
- (37) Hua Tong, Shuxin Ouyang, Yingpu Bi, **Naoto Umezawa**, Mitsutake Oshikiri, and Jinhua Ye, “Nano-photocatalytic Materials: Possibilities and Challenges”, *Adv. Mater.* **24**, 229-251, 2012.
- (36) Kui Xie, **Naoto Umezawa**, Ning Zhang, Pakpoom Reunchan, Yuanjian Zhang, and Jinhua Ye, “Self-doped SrTiO<sub>3-x</sub> photocatalyst with enhanced activity for artificial photosynthesis under visible light”, *Energy & Environmental Science* **4**, 4211-4219, 2011.
- (35) Katsumasa Kamiya, **Naoto Umezawa**, and Susumu Okada, “Energetics and electronic structure of graphene adsorbed on HfO<sub>2</sub> surface: Density functional theory calculations”, *Phys. Rev. B* **83** (15), 153413 (1-4), 2011.
- (34) Yingpu Bi, Shuxin Ouyang, **Naoto Umezawa**, Junyu Cao, and Jinhua Ye, “Facet effect of single-crystalline Ag<sub>3</sub>PO<sub>4</sub> Sub-microcrystals on Photocatalytic Properties”, *J. Am. Chem. Soc.* **133**, 6490-6492, 2011.
- (33) Hua Tong, **Naoto Umezawa**, Jinhua Ye, and Takahisa Ohno, “Electronic coupling assembly of semiconductor nanocrystals: self-narrowed band gap to promise solar energy utilization”, *Energy & Environmental Sci.* **4**, 1684-1689, 2011.
- (32) Hua Tong, **Naoto Umezawa**, and Jinhua Ye, “Visible light photoactivity from a bonding assembly of titanium oxide nanocrystals”, *Chem. Commun.* **47**, 4219-4221, 2011.
- (31) **Naoto Umezawa**, Ouyang Shuxin, and Jinhua Ye, “Theoretical study of high photocatalytic performance of Ag<sub>3</sub>PO<sub>4</sub>”, *Phys. Rev. B* **83** (3), 035202 (1-8), 2011.
- (30) **Naoto Umezawa** and Kenji Shiraishi, “Origin of high solubility of silicon in La<sub>2</sub>O<sub>3</sub>: A first-principles study”, *Appl. Phys. Lett.* **97** (20), 202906 (1-3), 2010.
- (29) **Naoto Umezawa**, “Effects of capping HfO<sub>2</sub> with multivalent oxides toward reducing the number of charged defects”, *Appl. Phys. Lett.* **96** (2), 162906 (1-3), 2010.
- (28) Hiroyoshi Momida, Eric Cockayne, **Naoto Umezawa**, and Takahisa Ohno, “Computational study of the dielectric properties of [La, Sc]<sub>2</sub>O<sub>3</sub> solid solutions”, *J. Appl. Phys.* **107** (7), 074104 (1-3), 2010.
- (27) Anderson Janotti, Joel B. Varley, Patrick Rinke, **Naoto Umezawa**, Georg Kresse, and Chris G. Van de Walle, “Hybrid functional studies of the oxygen vacancy in TiO<sub>2</sub>”, *Phys. Rev. B* **81** (8), 085212 (1-7), 2010.
- (26) **Naoto Umezawa**, “Effects of barium incorporation into HfO<sub>2</sub> gate dielectrics on reduction in charged defects: First-principles study”, *Appl. Phys. Lett.* **94** (2), 022903 (1-3), 2009.
- (25) **Naoto Umezawa**, Motoyuki Sato, and Kenji Shiraishi, “Reduction in charged defects associated with oxygen vacancies in hafnia by magnesium incorporation: First-principles study”, *Appl. Phys. Lett.* **93** (22), 223104 (1-3), 2008.

- (24) **Naoto Umezawa**, Kenji Shiraishi, Yasushi Akasaka, Atsushi Oshiyama, Seiji Inumiya, Seiichi Miyazaki, Kenji Ohmori, Toyohiro Chikyow, Takahisa Ohno, Kikuo Yamabe, Yasuo Nara, and Keisaku Yamada, “Chemical controllability of charge states of nitrogen-related defects in  $\text{HfO}_x\text{N}_y$ : First-principles calculations”, *Phys. Rev. B* **77** (16), 165130 (1-6), 2008.
- (23) **Naoto Umezawa**, Anderson Janotti, Patrick Rinke, Toyohiro Chikyow, and Chris G. Van de Walle, “Optimizing optical absorption of  $\text{TiO}_2$  by alloying with  $\text{TiS}_2$ ”, *Appl. Phys. Lett.* **92** (4), 041104 (1-3), 2008.
- (22) **Naoto Umezawa**, “Local-density approximation for orbital densities applied to the self-interaction correction”, *J. Chem. Phys.* **128** (4), 044105 (1-8), 2008.
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- (20) **Naoto Umezawa**, Kenji Shiraishi, Shinya Sugino, Akitomo Tachibana, Kenji Ohmori, Kuniyuki Kakushima, Hiroshi Iwai, Toyohiro Chikyow, Takahisa Ohno, Yasuo Nara, and Keisaku Yamada, “Suppression of oxygen vacancy formation in Hf-based high-k dielectrics by lanthanum incorporation”, *Appl. Phys. Lett.* **91** (13), 132904 (1-3), 2007.
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- (15) Rajendra Prasad, **Naoto Umezawa**, Dominik Domin, Romelia Salomon-Ferrer, and William A. Lester, Jr., “Quantum Monte Carlo study of first-row atoms using transcorrelated variational Monte Carlo trial functions”, *J. Chem. Phys.* **126** (16), 164109 (1-5), 2007.
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- (13) **Naoto Umezawa**, “Explicit Density Functional Exchange Potential with Correct Asymptotic Behavior”, *Phys. Rev. A* **74** (3), 032505 (1-7), 2006.
- (12) A. Uedono, T. Naito, T. Otsuka, K. Shiraishi, K. Yamabe, S. Miyazaki, H. Watanabe, **N. Umezawa**, T.

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- (10) **Naoto Umezawa** and Toyohiro Chikyow, "Role of the One-body Jastrow Factor in the Transcorrelated Self-consistent-field Equation", *Int. J. Quantum Chem.* **106** (7), 1477 – 1486, 2006.
- (9) Hiroyoshi Momida, Tomoyuki Hamada, Takenori Yamamoto, Tsuyoshi Uda, **Naoto Umezawa**, Toyohiro Chikyow, Kenji Shiraishi, and Takahisa Ohno, "Effect of nitrogen atom doping on dielectric constants of Hf-based gate oxides", *Appl. Phys. Lett.* **88** (11), 112903 (1-3), 2006.
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- (6) Heiji Watanabe, Satoshi Kamiyama, **Naoto Umezawa**, Kenji Shiraishi, Shiniti Yoshida, Yasumasa Watanabe, Tsunetoshi Arikado, Toyohiro Chikyow, Keisaku Yamada, and Kiyoshi Yasutake, "Role of nitrogen incorporation into Hf-based high-k gate dielectrics for termination of local current leakage paths", *Jpn. J. Appl. Phys.* **44** (43), L1333 – L1336, 2005.
- (5) **Naoto Umezawa**, Shinji Tsuneyuki, Takahisa Ohno, Kenji Shiraishi, and Toyohiro Chikyow, "A practical treatment for the three-body interactions in the transcorrelated variational Monte Carlo Method: application to atoms from lithium to neon", *J. Chem. Phys.* **122** (22), 224101 (1-9), 2005.
- (4) **Naoto Umezawa**, Kenji Shiraishi, Takahisa Ohno, Heiji Watanabe, Toyohiro Chikyow, Kazuyoshi Torii, Kikuo Yamabe, Keisaku Yamada, Hiroshi Kitajima, and Tsunetoshi Arikado, "First-Principles Studies of the Intrinsic Effect of Nitrogen Atoms on Reduction in Gate Leakage Current through Hf-based High-*k* Dielectrics", *Appl. Phys. Lett.* **86** (14), 143507 (1-3), 2005.
- (3) **Naoto Umezawa** and Shinji Tsuneyuki, "Excited electronic state calculations by the transcorrelated variational Monte Carlo method: Application to a helium atom", *J. Chem. Phys.* **121** (15), 7070 – 7075, 2004.
- (2) **Naoto Umezawa** and Shinji Tsuneyuki, "Ground-state correlation energy for the homogeneous electron gas calculated by the transcorrelated method", *Phys. Rev. B* **69** (16), 165102 (1-6), 2004.
- (1) **Naoto Umezawa** and Shinji Tsuneyuki, "Transcorrelated method for electronic systems coupled with variational Monte Carlo calculation", *J. Chem. Phys.* **119** (19), 10015 – 10031, 2003.

### **Invited talks**

- (14) **Naoto Umezawa** "Photocatalysts modeled with density-functional theory "Energy Material Nanotechnology, Spring Meeting, March 2014, Las Vegas, NV, USA
- (13) **Naoto Umezawa**, Adisak Boonchun, Pakpoom Reunchan, Shuxin Ouyang, and Junhua Ye, "Theoretical study of photocatalysis from defect, interface, and surface physics" International Union of Materials

Research Societies, September 2013, Qingdao, China

- (12) **Naoto Umezawa**, Pakpoom Reunchan, Shuxin Ouyang, Xu Hua, Yuanjian Zhang, and Jinhua Ye, “Theoretical Design of Highly Active SrTiO<sub>3</sub>-based Photocatalyst from Doping Scheme toward Solar Energy Utilization for Hydrogen Production”, 10th Pacific Rim Conference on Ceramic and Glass Technology, The American Ceramic Society, June 2013, San Diego, CA, USA
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- (1) **Naoto Umezawa**, Shinji Tsuneyuki, Takahisa Ohno, Atsushi Oshiyama, Kenji Shiraishi, and Toyohiro Chikyow, “Transcorrelated Approach for the Electronic State Calculations”, The 7<sup>th</sup> Asian Workshop on First-Principles Electronic Structure Calculations, November 2004, Taipei, Taiwan

## **Patents**

(1)

-Reference Number: 477(1)

-Control Number: 10W30USD

- Title: Method for reducing thickness of interfacial layer, method for



forming high dielectric constant gate insulating film, high dielectric constant gate insulating film, high dielectric constant gate oxide film, and transistor having high dielectric constant gate oxide film

- Inventor(s): Naoto Umezawa, Toyohiro Chikyo, Toshihide Nabatame

- Applicant(s): National Institute for Materials Science (NIMS)

- Patent Application No. 14/046339

- Patent Registration No. 8759925

- Patent Filing Date: 2010 November 30

- Patent Registration Date: 2014 June 24

(2)

-Reference Number: US519

-Control Number: 11MS013US

- Title: Transparent electric conductor

- Inventor(s): Toyohiro Chikyow, Seunghwan Park, Naoto Umezawa//Laura Jane Singh, David Nicolas

- Applicant(s): National Institute for Materials Science (NIMS)//Saint-Gobain Glass France

- Patent Application No. US14/113,774

- Patent Filing Date: 2012 April 26

***Updated on November, 2015***