

2012

- [1] Akitomo Tachibana,
“General relativistic symmetry of electron spin torque”,
Journal of Mathematical Chemistry, 50, 669-688, (2012)
DOI: 10.1007/s10910-011-9943-z
- [2] Kazuhide Ichikawa, Yuji Ikeda, Ryo Terashima and Akitomo Tachibana,
“Aluminum Hydride Clusters as Hydrogen Storage Materials and their Electronic Stress Tensor Analysis”,
Proceedings for THERMEC’ 2011
Materials Science Forum Vols. 706-709 (2012) 1539-1544
doi:10.4028/www.scientific.net/MSF.706-709.1539
- [3] Masato Senami, Yasushi Tsuchida, Akinori Fukushima, Yuji Ikeda, Akitomo Tachibana,
“Local Dielectric Property of Cubic, Tetragonal, and Monoclinic Hafnium Oxides”,
Japanese Journal of Applied Physics, 51, 031101(11), (2012)
[DOI:10.1143/JJAP.51.031101](https://doi.org/10.1143/JJAP.51.031101)
- [4] Takaaki Hara, Masato Senami, Akitomo Tachibana,
“Electron spin torque in atoms”,
Physics Letters A, 376, 1434-1441, (2012)
[DOI:10.1016/j.physleta.2012.03.028](https://doi.org/10.1016/j.physleta.2012.03.028)
- [5] Kazuhide Ichikawa, Masahiro Fukuda and Akitomo Tachibana,
“Study of Simulation Method of Time Evolution in Rigged QED”,
International Journal of Quantum Chemistry, published online.
DOI: 10.1002/qua.24087
- [6] Akitomo Tachibana,
“Electronic Stress with Spin Vorticity”,
Frontiers in Theoretical Chemistry: Concepts and Methods: A tribute to Professor B.M. Deb; Eds. by Swapan K.Ghosh and Pratim K.Chattaraj;
Taylor & Francis / CRC Press, 2012; Chapter XXX, pp.xxx-xxx

2011

- [1] Masato Senami, Yuji Ikeda, and Akitomo Tachibana, "Local Transport Property of GaN Cluster as a Model of Nanowire",
Japanese Journal of Applied Physics, 50, 010103(7), (2011)
(Selected Topics in Applied Physics (STAP))
- [2] D. J. Henry, P. Szarek, K. Hirai, K. Ichikawa, A. Tachibana and I. Yarovsky,
"Reactivity and Regioselectivity of Aluminum Nanoclusters: Insights from Regional Density Functional Theory",
Journal of Physical Chemistry C, 115(5), 1714-1723 (2011)
- [3] Kazuhide Ichikawa, Yuji Ikeda, Ayumu Wagatsuma, Kouhei Watanabe, Pawel Szarek and Akitomo Tachibana
"Theoretical study of hydrogenated tetrahedral aluminum clusters"
International Journal of Quantum Chemistry, 111, 3548-3555 (2011)
DOI: 10.1002/qua.22848
- [4] Masato Senami, Y. Ikeda, Takaaki Hara, and Akitomo Tachibana,
"Nanosize Electronics Material Analysis by Local Quantities Based on the Rigged QED",
Key Engineering Materials, Vol. 470, pp. 66-71, (2011)
- [5] Akinori Fukushima, Akira Sawairi, Kentaro Doi, Masato Senami, Liang Chen, Hansong Cheng, and Akitomo Tachibana,
"Role of an Aluminum atom on Graphene for Hydrogen Adsorption",
Journal of Physical Society of Japan, 80, 074705 (9), (2011)
[DOI:10.1143/JPSJ.80.074705](https://doi.org/10.1143/JPSJ.80.074705)
- [6] Kazuhide Ichikawa, Ayumu Wagatsuma, Yusaku I. Kurokawa, Shigeyoshi Sakaki, Akitomo Tachibana,
"Inverted-sandwich-type and open-lantern-type dinuclear transition metal complexes: theoretical study of chemical bonds by electronic stress tensor",
Theoretical Chemistry Accounts, 130:237-250 (2011)
DOI: 10.1007/s00214-011-0966-0
- [7] Yuji Ikeda, Norifumi Ohmori, Noriaki Maida, Masato Senami, Akitomo Tachibana,
"Theoretical study of gallium nitride crystal growth reaction mechanism",

Japanese Journal of Applied Physics, 50, 125601(7), (2011)

[DOI:10.1143/JJAP.50.125601](https://doi.org/10.1143/JJAP.50.125601)

[8] Masato Senami, Yuji Ikeda, Akinori Fukushima, Akitomo Tachibana,
“Theoretical study of adsorption of lithium atom on carbon nanotube”,
AIP Advances, 1, 042106(12), (2011)

[doi:10.1063/1.3651182](https://doi.org/10.1063/1.3651182)

[9] Kazuhide Ichikawa, Ayumu Wagatsuma, Pawel Szarek, Chenggang Zhou, Hansong
Cheng, Akitomo Tachibana,
“Electronic stress tensor analysis of hydrogenated palladium clusters”,
Theoretical Chemistry Accounts, 130:531-542 (2011)

DOI: 10.1007/s00214-011-1044-3

2010

- [1] P. Szarek, K. Watanabe, K. Ichikawa, and A. Tachibana
“Electronic stress tensor study of aluminum nanostructures for hydrogen storage”
Proceedings for THERMEC’ 2009
Materials Science Forum Vols. 638-642 (2010) 1137-1142
- [2] A. Tachibana
"Energy density concept: A stress tensor approach"
Journal of Molecular Structure: THEOCHEM 943, 138-151 (2010)
- [3] K. Ichikawa, A. Wagatsuma, M. Kusumoto and A. Tachibana
“Electronic stress tensor of the hydrogen molecular ion: Comparison between the exact wave function and approximate wave functions using Gaussian basis sets”
Journal of Molecular Structure: THEOCHEM 951, 49-59 (2010)
- [4] Akinori Fukushima, Kosuke Hirai, Masato Senami, Akitomo Tachibana,
"Theoretical study of the migration of the hydrogen atom adsorbed on aluminum nano wire"
Surface Science 604, 1718-1726 (2010)
- [5] Masato SENAMI, Jun NISHIKAWA, Takaaki HARA, and Akitomo TACHIBANA,
"Spin Torque and Zeta Force of Dimer of Alkali Atoms",
Journal of the Physical Society of Japan, 79, 084302(9), (2010)
- [6] Akinori Fukushima, Masato Senami, Yasushi Tsuchida, and Akitomo Tachibana,
"Local Dielectric Property of Cubic Hafnia",
Japanese Journal of Applied Physics, 49, 111504(7), (2010)
- [7] Masato Senami, Yuji Ikeda, Akinori Fukushima, and Akitomo Tachibana,
"Calculation of the electronic state in electronic current for nanowire models",
Japanese Journal of Applied Physics, 49, 115002(5), (2010)
- [8] Akinori Fukushima, Shinya Sugino, Yasushi Tsuchida, Masato Senami, and Akitomo Tachibana,
“Local Dielectric Property of Hafnium and Lanthanum Atoms in HfLaO_x ”,
Japanese Journal of Applied Physics, 49, 121504(11), (2010)

2009

- [1] K. Matsumoto, H. Tokunaga and A. Tachibana
“MOCVD Growth of GaN and Related Materials,”
Oxide and Nitride Semiconductors Processing, Properties and Applications Series, ed.
by Y. Takafumi, H. Soon-Ku (Springer, 2009) Vol. 12, Chapter 3.2 pp. 130-155.
- [2] Paweł Szarek, Kousuke Urakami, Chenggang Zhou, Hansong Cheng and Akitomo Tachibana
“On reversible bonding of hydrogen molecules on platinum clusters,”
J. Chem. Phys., **130**, 084111 (2009).
- [3] P. Szarek, K. Hirai, K. Ichikawa, D. Henry, I. Yarovsky, and A. Tachibana
“Regional DFT --- Electronic Stress Tensor Study of Aluminum Nanostructures for Hydrogen Storage”
AIP Conf. Proc. **1102**, 299-305 (2009)
- [4] K. Ichikawa, T. Myoraku, A. Fukushima, Y. Ishihara, R. Isaki, T. Takeguchi and A. Tachibana
“A Theoretical Study on a Reaction of Iron(III) Hydroxide with Boron Trichloride by Ab Initio Calculation”
Journal of Molecular Structure: THEOCHEM 915, 1-10 (2009)
- [5] K. Ichikawa and A. Tachibana
“Stress tensor of the hydrogen molecular ion”
Phys. Rev. A80, 062507(4) (2009).

2008

[1] Kentaro Doi, Yutaka Mikazuki, Shinya Sugino, Tatsuki Doi, Pawel Szarek, Masato Senami, Kenji Shiraishi, Hiroshi Iwai, Naoto Umezawa, Toyohiro Chikyo, Keisaku Yamada, and Akitomo Tachibana,

"Electronic Structure Study of Local Dielectric Properties of Lanthanoid Oxide Clusters,"

Jpn. J. Appl. Phys., **47**, 205-211 (2008); errata, Ph.D. thesis, Pawel Szarek, 京都大学学術情報リポジトリ (京都大学図書館機構) Szarek, Pawel. Theoretical Study of Electronic States of Chemical Bonds.

(化学結合の電子状態に関する理論的研究.)

<http://hdl.handle.net/2433/66212>

[2] Chenggang Zhou, Shujuan Yao, Jinping Wu, Robert Forrey, Liang Chen, Akitomo Tachibana, and Hansong Cheng,

"Hydrogen dissociative chemisorption and desorption on saturated subnano palladium clusters (Pd_n, n = 2–9),"

Phys. Chem. Chem. Phys., **10**, 5445-5451 (2008).

[3] Akinori Fukushima, Kentaro Doi, Masato Senami, and Akitomo Tachibana, "Theoretical study for AlB nanowire as hydrogen adsorption material",

J. Power Sources **184**, 60-76 (2008).

[4] Pawel Szarek, Yutaka Sueda and Akitomo Tachibana,

"Electronic stress tensor description of chemical bonds using nonclassical bond order concept,"

J. Chem. Phys. **129**, 094102-1-16 (2008).

[5] Pawel Szarek, Edyta Dyguda-Kazimierowicz, Akitomo Tachibana, W. Andrzej Sokalski,

"Physical Nature of Intermolecular Interactions within cAMP-Dependent Protein Kinase Active Site: Differential Transition State Stabilization in Phosphoryl Transfer Reaction,"

J. Phys. Chem. B, **112** (37), 11819–11826 (2008).

2007

[1] Piotr Ordon and Akitomo Tachibana,

“Use of nuclear stiffness in search for a maximum hardness principle and for the softest states along the chemical reaction path: A new formula for the energy third derivative γ ”

J. Chem. Phys., **126**, 234115-1-11, (2007).

[2] Pawel Szarek and Akitomo Tachibana,

“The field theoretical study of chemical interaction in terms of the Rigged QED: new reactivity indices,”

J. Mol. Model., **13**, 651-663 (2007).

[3] Kentaro Doi, Noriaki Maida, Kotaro Kimura, and Akitomo Tachibana,

“First-principle study on crystal growth of Ga and N layers on GaN substrate,”

Physica Stat. Sol. C 4, No. 7, 2293-2296 (2007).

[4] Kentaro Doi, Hiroshi Nakano, Hirokazu Ohta, and Akitomo Tachibana,

“First-principle molecular-dynamics study of hydrogen and aluminum nanowires in carbon nanotubes,”

Mater Sci. Forum **539-543**, 1409-1414 (2007).

[5] Hiroshi Nakano, Pawel Szarek, Kentaro Doi, and Akitomo Tachibana,

"Theoretical studies of the transition states along the reaction coordinates of [Ni Fe] hydrogenase,"

in Molecular Materials with Specific Interactions-Modeling and Design, Challenges and Advances in Computational Chemistry and Physics, Vol. 4, Series Editor J. Leszczynski, Ed. by W. Andrzej Sokalski (Springer, Dordrecht, The Netherlands, 2007), Chapter 9, pp. 399-432.

[6] Naoto Umezawa, Kenji Shiraishi, Shinya Sugino, Akitomo Tachibana, Kenji Ohmori, Kuniyuki Kakushima, Hiroshi Iwai, Toyohiro Chikyo, T. Ohno, Yasuo Nara, and Keisaku Yamada,

“Suppression of Oxygen Vacancy Formation in Hf-based High-k Dielectrics by Lanthanum Incorporation,”

Appl. Phys. Lett. **91**, 132904 (2007).

[7] Chenggang Zhou, Jinping Wu, Aihua Nie, Robert C. Forrey, Akitomo Tachibana, and

Hansong Cheng,

“On the Sequential Hydrogen Dissociative Chemisorption on Small Platinum Clusters: A Density Functional Theory Study,”

J. Phys. Chem. C, **111**, 12773-12778 (2007).

2006

[1] Hiroshi Nakano, Hirokazu Ohta, Akira Yokoe, Kentaro Doi, and Akitomo Tachibana,
“First-principle molecular-dynamics study of hydrogen adsorption on an aluminum-doped
carbon nanotube,”
J. Power Sources **163**, 125-134 (2006).

[2] Kentaro Doi, Koichi Nakamura, and Akitomo Tachibana,
“Local-property analysis for modeling of gate insulator materials,”
Nano CMOS, 2006 International Workshop on, (IEEE 2006), pp. 209-235

2005

[1] Akitomo Tachibana,

“A new visualization scheme of chemical energy density and bonds in molecules,”

J. Mol. Model. **11**(4), 301-311 (2005).

[2] Piotr Ordon and Akitomo Tachibana,

“Nuclear reactivity indices within regional density functional theory,”

J. Mol. Model. **11**(4), 312-316 (2005).

[3] Piotr Ordon and Akitomo Tachibana,

“Investigation of the role of the C-PCM solvent effect in reactivity indices,”

J. Chem. Sci. **117**(4), 583-589 (2005).

[4] Koichi Nakamura, Kentaro Doi, Kiwamu Fujitani, and Akitomo Tachibana,

“Theoretical study on the first-principle dielectric properties of silicate compounds,”

Phys. Rev. B **71**(4), 045332-1-045332-8 (2005).

[5] Kentaro Doi, Kiwamu Fujitani, Naoki Kadowaki, Koichi Nakamura, Akitomo Tachibana, and Takeo Hattori,

“Structures and electronic states of gadolinium oxide clusters,”

Jpn. J. Appl. Phys. **44**, 6115-6123 (2005).

[6] Naoomi Ibuta, Fuihiko Sagara, Kentaro Doi, Koichi Nakamura, Akitomo Tachibana, Yoshio Ishihara, and Katsumasa Suzuki,

“Reaction processes of germane molecules with catalytic water,”

Jpn. J. Appl. Phys. **44**, 4133-4141 (2005).

[7] Kentaro Doi, Koichi Yoshida, Hiroshi Nakano, Akitomo Tachibana, Takahisa Tanabe, Yuko Kojima, and Keiji Okazaki,

“Ab initio calculation of electron effective masses in solid pentacene,”

J. Appl. Phys. **98**, 113709-1-113709-7 (2005).

2004

[1] Akitomo Tachibana,

“Spindle structure of the stress tensor of chemical bond,”

Int. J. Quant. Chem. **100**, 981-993 (2004).

[2] Yoshihiko Kawakami, Yaichi Nojima, Kentaro Doi, Koichi Nakamura, and Akitomo Tachibana, “First-principle study on structures and electronic properties of aluminum nanowire wrapped in carbon nanotube,”

Electrochim. Acta **50**, 739-744 (2004).

[3] Kentaro Doi, Nobuyuki Higashimaki, Yoshihiko Kawakami, Koichi Nakamura, and Akitomo Tachibana,

“First-principle study on electronic properties of gallium nitride and aluminum nitride nanowires,”

Phys. Stat. Sol. B **241(12)**, 2806-2810 (2004).

[4] Takanobu Okada, Kentaro Doi, Koichi Nakamura, and Akitomo Tachibana,

“Quantum chemical study on substituent effect of gas-phase reactions in III-V nitride semiconductor crystal growth,”

Phys. Stat. Sol. B **241(12)**, 2744-2748 (2004).

[5] Koh Matsumoto and Akitomo Tachibana,

“Growth mechanism of atmospheric pressure MOVPE of GaN and its alloys: gas phase chemistry and its impact on reactor design,”

J. of Cryst. Growth **272(1-4)**, 360-369 (2004).