<u>2007</u>

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

in Molecular Materials with Specific Interactions-Modeling and Design, Challeng es and Advances in Computational Chemistry and Physics, Vol. 4, Series Editor J. Leszczynski, Ed. by W. Andrzey Sokalski (Springer, Dordrecht, The Nether lands, 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).