2001

" Electronic energy density in chemical reaction systems," A. Tachibana, Journal of Chemical Physics,**115**, 3497-3518 (2001).

"Ion-Specificity for Hydrogen-Bonding Hydration of Polymer: An Approach by Ab Initio Molecular Orbital Calculations," H. Muta, R. Kojima, S. Kawauchi, A. Tachibana, and M. Satoh, J. Mol. Structure (Theochem), **536**, 219-226 (2001).

" First-principle theoretical study on epitaxial crystal growth of GaN," M. Murata, M. Ikenaga, K. Nakamura, A. Tachibana and K. Matsumoto, phys. stat. sol. (a) **188**, 579-582 (2001).

" First-Principle Theoretical Study on Reliability of SiO_2 Thin Films under External Electric Field,
" Kentaro Doi, Koichi Nakamura and Akitomo Tachibana, in *Extended Abstracts of International Workshop on Gate Insulator 2001*, Eds. by S. Ohmi et al. (Business Center for Academic Societies Japan, Tokyo, 2001), pp. 148-151.

"First-Principle Electronic Properties of ZrO_2 and HfO_2 Crystals under External Electric Field, " Shin Egami, Koichi Nakamura and Akitomo Tachibana, in *Extended Abstracts of International Workshop on Gate Insulator 2001*, Eds. by S. Ohmi et al. (Business Center for Academic Societies Japan, Tokyo, 2001), pp. 234-237.