

Theory Papers

Kitaura, K.; Sawai, T.; Asada, T.; Nakano, T.; Uebayasi, M. *Chem. Phys. Lett.* **1999**, *312*, 319.

Kitaura, K.; Ikeo, E.; Asada, T.; Nakano, T.; Uebayasi, M. *Chem. Phys. Lett.* **1999**, *313*, 701.

Nakano, T.; Kaminuma, T.; Sato, T.; Akiyama, Y.; Uebayasi, M.; Kitaura, K. *Chem. Phys. Lett.* **2000**, *318*, 614

Kitaura, K.; Sugiki, S.-I.; Nakano, T.; Komeiji, Y.; Uebayasi, M. *Chem. Phys. Lett.* **2001**, *336*, 163.

Inadomi, Y.; Nakano, T.; Kitaura, K.; Nagashima, U. *Chem. Phys. Lett.* **2002**, *364*, 139.

Nakano, T.; Kaminuma, T.; Sato, T.; Fukuzawa, K.; Akiyama, Y.; Uebayasi, M.; Kitaura, K. *Chem. Phys. Lett.* **2002**, *351*, 475.

Fedorov, D. G.; Kitaura, K. *J. Phys. Chem. A* **2007**, *111*, 6904.

Mochizuki, Y.; Yamashita, K.; Murase, T.; Nakano, T.; Fukuzawa, K.; Takematsu, K.; Watanabe, H.; Tanaka, S. *Chem. Phys. Lett.* **2008**, *457*, 396.

Fedorov, D. G., Kitaura, K. *J. Chem. Phys.* **2004**, *120*, 6832.

Fedorov, D. G.; Kitaura, K. *Chem. Phys. Lett.* **2004**, *389*, 129.

Fedorov, D. G.; Kitaura, K. *J. Chem. Phys.* **2004**, *121*, 2483.

Yasuda, Y.; Yamaki, K. *J. Chem. Phys.* **2006**, *125*, 154101.

Fedorov, D.G.; Kitaura, K. *J. Chem. Phys.* **2005**, *123*, 134103.

D. G. Fedorov, D.G.; Jensen, J.H.; Deka, R.C.; Kitaura, K. *J. Phys. Chem. A* **2008**, *112*, 11808.

Fedorov, D. G.; Kitaura, K. *J. Comp. Chem.* **2007**, *28*, 222.

Fedorov, D.G.; Kitaura, K. *Chem. Phys. Lett.* **2006**, *433*, 182.

M. Chiba, D. G. Fedorov, K. Kitaura, *Chem. Phys. Lett.* 444 (2007) 346-350

M. Chiba, D. G. Fedorov, K. Kitaura, *J. Chem. Phys.* 127 (2007) 104108

D. G. Fedorov, K. Kitaura, *J. Comp. Chem.* 28 (2007) 222-237

Application Papers

Fedorov, D. G.; Kitaura, K. In *Modern Methods for Theoretical Physical Chemistry and Biopolymers*; Starikov, E. B., Lewis, J. P., Tanaka, S., Eds.; Elsevier: Amsterdam, 2006; pp 3-38

Nakano, T.; Mochizuki, Y.; Fukuzawa, K.; Amari, S.; Tanaka, S. In *Modern Methods for Theoretical Physical Chemistry and Biopolymers*; Starikov, E. B., Lewis, J. P., Tanaka, S., Eds.; Elsevier: Amsterdam, 2006; pp 39-52

Goto, H.; Obata, S.; Kamakura, T.; Nakayama, N.; Sato, M.; Nakajima, Y.; Nagashima, U.; Watanabe, T.; Inadomi, Y.; Ito, M.; Nishikawa, T.; Nakano, T.; Nilsson, L.; Tanaka, S.; Fukuzawa, K.; Inagaki, Y.; Hamada, M.; Chuman, H. In *Modern Methods for Theoretical Physical Chemistry and Biopolymers*; Starikov, E. B., Lewis, J. P., Tanaka, S., Eds.; Elsevier: Amsterdam, 2006; pp 227-248

Parallelized integral-direct CIS(D) calculations with multilayer fragment molecular orbital scheme, Y. Mochizuki, K. Tanaka, K. Yamashita, T. Ishikawa, T. Nakano, S. Amari, K. Segawa, T. Murase, H. Tokiwa, M. Sakurai, *Theor. Chem. Acc.* 117 (2007) 541-553

The Fragment Molecular Orbital Method for Geometry Optimizations Polypeptides and Proteins, D. G. Fedorov, T. Ishida, M. Uebayasi, K. Kitaura, *J. Phys. Chem. A* 111 (2007) 2722-2732

Change in a protein's electronic structure induced by an explicit solvent: An ab initio fragment molecular orbital study of ubiquitin, Y. Komeiji, T. Ishida, D. G. Fedorov, K. Kitaura, *J. Comp. Chem.* 28 (2007) 1750-1762

Fragmentation Method Combined with Quantum Monte Carlo Calculations, R. Maezono, H. Watanabe, S. Tanaka, M. D. Towler, R. J. Needs, *J. Phys. Soc. Jap.* 76 (2007) 064301

Fedorov, D. G.; Ishimura, K.; Ishida, T.; Kitaura, K.; Pulay, P.; Nagase, S. *J. Comp. Chem.* 2007, 28, 1476

Dahlke, E. E.; Truhlar, D. G. *J. Chem. Theor. Comput.* 2007, 3, 46

Watanabe, T., Inadomi, Y., Fukuzawa, K., Nakano, T., Tanaka, S., Nilsson, L., Nagashima, U. *J. Phys. Chem. B* 2007, 111, 9621

Okuyama, Y., Watanabe, T., Fukuzawa, K., Nakano, T., Mochizuki, Y., Ishikawa, T., Tanaka, S., Ebina, K. Chem. Phys. Lett. 2007, 449, 7

Fedorov, D. G., Ishimura, K., Ishida, T., Kitaura, K., Pulay, P., Nagase S. 2007. Accuracy of the three-body fragment molecular orbital method applied to Møller-Plesset perturbation theory. J. Comput. Chem. 28:1476-1484

Chiba, M., Fedorov, D. G., Kitaura, K. 2007. Time-dependent density functional theory with the multilayer fragment molecular orbital method. Chem. Phys. Lett. 444:346-350

Gao, Q., Yokojima, S., Kohno, T. et al. 2007. Ab initio NMR chemical shift calculations on proteins using fragment molecular orbitals with electrostatic environment. Chem. Phys. Lett. 445:331-339

Ishikawa, T., Mochizuki, Y., Amari, S. et al. 2007. Fragment interaction analysis based on local MP2. Theor. Chem. Acc. 118:937-945

Maezono, R., Watanabe, H., Tanaka, S., Towler, M. D., Needs, R. J. 2007. Fragmentation method combined with quantum Monte Carlo calculations. J. Phys. Soc. Jap. 76:064301

Watanabe, H., Enomoto, T., Tanaka, S. 2007. Ab initio study of molecular interactions in higher plant and *Galdieria partita* Rubiscos with the fragment molecular orbital method. Biochem. Biophys. Res. Comm. 361:367-372

Mochizuki, Y., Yamashita, K., Murase, T., Nakano, T., Fukuzawa, K., Takematsu, K., Watanabe, H., Tanaka, S. Chem. Phys. Lett. 2008, 457, 396

Ito, M., Fukuzawa, K., Mochizuki, Y., Nakano, T., Tanaka, S. 2008. Ab initio fragment molecular orbital study of molecular interactions between liganded retinoid X receptor and its coactivator; part II: influence of mutations in transcriptional activation function 2 activating domain core on the molecular interactions. J. Phys. Chem. A 112:1986-1998

Iwata, T., Fukuzawa, K., Nakajima, K. et al. 2008. Theoretical analysis of binding specificity of influenza viral hemagglutinin to avian and human receptors based on the fragment molecular orbital method. Comput. Biol. Chem. 32:198-211

Harada, T., Yamagishi, K., Nakano, T., Kitaura, K., Tokiwa, H. 2008. Ab initio fragment molecular orbital study of ligand binding to human progesterone receptor ligand-binding domain. Naunyn-Schmiedeberg's Arch. Pharmac. 377:607-615

Large scale FMO-MP2 calculations on a massively parallel-vector computer, Y. Mochizuki, K. Yamashita, T. Murase, T. Nakano, K. Fukuzawa, K. Takematsu, H. Watanabe, S. Tanaka, Chem. Phys. Lett. 457 (2008) 396-403

Sawada, T., Hashimoto, T., Tokiwa, H. et al. 2008. Ab initio fragment molecular orbital studies of influenza virus hemagglutinin-sialosaccharide complexes toward chemical clarification about the virus host range determination. *Glycoconj. J.*, in press

Ozawa, T., Okazaki, K. 2008. CH/π hydrogen bonds determine the selectivity of the Src homology 2 domain to tyrosine phosphotyrosyl peptides: an ab initio fragment molecular orbital study. *J. Comput. Chem.*, in press

Review Articles

Extending the Power of Quantum Chemistry to Large Systems with the Fragment Molecular Orbital Method, D. G. Fedorov, K. Kitaura, *J. Phys. Chem. A* 111 (2007) 6904-6914

Accurate Methods for Large Molecular Systems, M.S. Gordon, J.M. Mullin, S.R. Pruitt, L.B. Roskop, L.V. Slipchenko, J.A. Boatz, *J. Phys. Chem. B* 113 (2009) 9646-9663