

# Shigenori Tanaka

## List of Publications by Year in Descending Order

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The third column is the impact factor (IF) of the journal, and the fourth column is the number of citations of the article.

143  
papers

3,118  
citations

33  
h-index

48  
g-index

162  
ext. papers

3,419  
ext. citations

3.2  
avg, IF

5.35  
L-index

| #   | Paper  | IF  | Citations |
|-----|--|-----|-----------|
| 143 | Remarkable Suppression of Allosteric Protomer-Protomer Dissociation Reaction Elucidated by Molecular Dynamics Simulation. <i>Proteins: Structure, Function and Bioinformatics</i> , <b>2022</b> ,  | 4.2 | 1         |
| 142 | Collective residue interactions in trimer complexes of SARS-CoV-2 spike proteins analyzed by fragment molecular orbital method. <i>Applied Physics Express</i> , <b>2022</b> , 15, 017001  | 2.4 | 2         |
| 141 | Quantum Brain Dynamics in 2+1 dimensions: Non-equilibrium analysis towards memory formations. <i>Physica A: Statistical Mechanics and Its Applications</i> , <b>2022</b> , 598, 127397   | 3.3 |           |
| 140 | Elucidating microscopic events driven by GTP hydrolysis reaction in the Ras-GAP system with semi-reactive molecular dynamics simulations: the alternative role of a phosphate binding loop for mechanical energy storage. <i>Physical Chemistry Chemical Physics</i> , <b>2021</b> , 23, 26151-26164 | 3.6 | 1         |
| 139 | Fragment molecular orbital calculations for biomolecules. <i>Current Opinion in Structural Biology</i> , <b>2021</b> , 72, 127-134   | 8.1 | 3         |
| 138 | In silico modeling of PAX8-PPAR $\gamma$ fusion protein in thyroid carcinoma: influence of structural perturbation by fusion on ligand-binding affinity. <i>Journal of Computer-Aided Molecular Design</i> , <b>2021</b> , 35, 629-642   | 4.2 |           |
| 137 | Appearance of Thermal Time. <i>Foundations of Physics</i> , <b>2021</b> , 51,  | 1.2 | 1         |
| 136 | Non-equilibrium Quantum Brain Dynamics II: Formulation in 3+1 dimensions. <i>Physica A: Statistical Mechanics and Its Applications</i> , <b>2021</b> , 567, 125706   | 3.3 | 2         |
| 135 | Density-Matrix Based Scheme of Basis Selection for Linear Combination of Fragment Molecular Orbitals. <i>Journal of the Physical Society of Japan</i> , <b>2021</b> , 90, 064301   | 1.5 |           |
| 134 | Dynamic Cooperativity of Ligand-Residue Interactions Evaluated with the Fragment Molecular Orbital Method. <i>Journal of Physical Chemistry B</i> , <b>2021</b> , 125, 6501-6512   | 3.4 | 8         |
| 133 | Comparison of Various Fragmentation Methods for Quantum Chemical Calculations of Large Molecular Systems <b>2021</b> , 15-27   |     |           |
| 132 | The ABINIT-MP Program <b>2021</b> , 53-67  |     | 2         |
| 131 | Fragment Molecular Orbital Method as Cluster Expansion <b>2021</b> , 3-14  |     |           |
| 130 | FMODB: The World's First Database of Quantum Mechanical Calculations for Biomacromolecules Based on the Fragment Molecular Orbital Method. <i>Journal of Chemical Information and Modeling</i> , <b>2021</b> , 61, 777-794   | 6.1 | 11        |
| 129 | Statistical interaction analyses between SARS-CoV-2 main protease and inhibitor N3 by combining molecular dynamics simulation and fragment molecular orbital calculation. <i>Applied Physics Express</i> , <b>2021</b> , 14, 027003  | 2.4 | 10        |
| 128 | Interaction analyses of SARS-CoV-2 spike protein based on fragment molecular orbital calculations. <i>RSC Advances</i> , <b>2021</b> , 11, 3272-3279   | 3.7 | 11        |
| 127 | Molecular recognition of SARS-CoV-2 spike glycoprotein: quantum chemical hot spot and epitope analyses. <i>Chemical Science</i> , <b>2021</b> , 12, 4722-4739  | 9.4 | 22        |

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| 126 | Reaction Pathway Sampling and Free-Energy Analyses for Multimeric Protein Complex Disassembly by Employing Hybrid Configuration Bias Monte Carlo/Molecular Dynamics Simulation. <i>ACS Omega</i> , <b>2021</b> , 6, 4749-4758                            | 3.9 | 1  |
| 125 | Fragment molecular orbital based interaction analyses on complexes between SARS-CoV-2 RBD variants and ACE2. <i>Japanese Journal of Applied Physics</i> , <b>2021</b> , 60, 090901   | 1.4 | 3  |
| 124 | FMO Drug Design Consortium <b>2021</b> , 127-181   |     | 1  |
| 123 | Fragment Molecular Orbital Based Interaction Analyses on COVID-19 Main Protease - Inhibitor N3 Complex (PDB ID: 6LU7). <i>Journal of Chemical Information and Modeling</i> , <b>2020</b> , 60, 3593-3602   | 6.1 | 50 |
| 122 | Nanoscale Quantum Thermal Conductance at Water Interface: Green@ Function Approach Based on One-Dimensional Phonon Model. <i>Molecules</i> , <b>2020</b> , 25,   | 4.8 | 1  |
| 121 | Identification of correlated inter-residue interactions in protein complex based on the fragment molecular orbital method. <i>Journal of Molecular Graphics and Modelling</i> , <b>2020</b> , 100, 107650  | 2.8 | 11 |
| 120 | New Modified Deoxythymine with Dibranching Tetraethylene Glycol Stabilizes G-Quadruplex Structures. <i>Molecules</i> , <b>2020</b> , 25,   | 4.8 | 3  |
| 119 | Strongly coupled electron liquid: Ab initio path integral Monte Carlo simulations and dielectric theories. <i>Physical Review B</i> , <b>2020</b> , 101,   | 3.3 | 22 |
| 118 | Temperature relaxation in binary hard-sphere mixture system: Molecular dynamics and kinetic theory study. <i>Journal of Chemical Physics</i> , <b>2020</b> , 153, 034114   | 3.9 | 0  |
| 117 | Machine learning prediction of inter-fragment interaction energies between ligand and amino-acid residues on the fragment molecular orbital calculations for Janus kinase inhibitor complex. <i>Chemical Physics Letters</i> , <b>2020</b> , 757, 137883 | 2.5 | 2  |
| 116 | Comparative study on model parameter evaluations for the energy transfer dynamics in Fenna-Matthews-Dixon complex. <i>Chemical Physics</i> , <b>2020</b> , 539, 110903   | 2.3 | 3  |
| 115 | Nonequilibrium quantum brain dynamics. <i>Advances in Quantum Chemistry</i> , <b>2020</b> , 82, 159-180  | 1.4 | 1  |
| 114 | Effective Static Approximation: A Fast and Reliable Tool for Warm-Dense Matter Theory. <i>Physical Review Letters</i> , <b>2020</b> , 125, 235001  | 7.4 | 24 |
| 113 | Taking Water into Account with the Fragment Molecular Orbital Method. <i>Methods in Molecular Biology</i> , <b>2020</b> , 2114, 105-122  | 1.4 | 6  |
| 112 | Development of an automated fragment molecular orbital (FMO) calculation protocol toward construction of quantum mechanical calculation database for large biomolecules. <i>Chem-Bio Informatics Journal</i> , <b>2019</b> , 19, 5-18                    | 0.8 | 18 |
| 111 | Non-Equilibrium Quantum Electrodynamics in Open Systems as a Realizable Representation of Quantum Field Theory of the Brain. <i>Entropy</i> , <b>2019</b> , 22,  | 2.8 | 1  |
| 110 | Non-Equilibrium Quantum Brain Dynamics: Super-Radiance and Equilibration in 21 Dimensions+. <i>Entropy</i> , <b>2019</b> , 21, 1066  | 2.8 | 3  |
| 109 | ATP Converts A $\beta$ Oligomer into Off-Pathway Species by Making Contact with Its Backbone Atoms Using Hydrophobic Adenosine. <i>Journal of Physical Chemistry B</i> , <b>2019</b> , 123, 9922-9933  | 3.4 | 9  |

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| 108 | Fragment Molecular Orbital Calculations with Implicit Solvent Based on the Poisson-Boltzmann Equation: II. Protein and Its Ligand-Binding System Studies. <i>Journal of Physical Chemistry B</i> , <b>2019</b> , 123, 957-973   | 3.4  | 34 |
| 107 | Ab initio molecular dynamics study of prebiotic production processes of organic compounds at meteorite impacts on ocean. <i>Journal of Computational Chemistry</i> , <b>2019</b> , 40, 349-359  | 3.5  | 3  |
| 106 | Application of singular value decomposition to the inter-fragment interaction energy analysis for ligand screening. <i>Computational and Theoretical Chemistry</i> , <b>2018</b> , 1132, 23-34  | 2    | 17 |
| 105 | Fragment Molecular Orbital Calculations with Implicit Solvent Based on the Poisson-Boltzmann Equation: Implementation and DNA Study. <i>Journal of Physical Chemistry B</i> , <b>2018</b> , 122, 4457-4471  | 3.4  | 28 |
| 104 | Computational Analysis of the Interaction Energies between Amino Acid Residues of the Measles Virus Hemagglutinin and Its Receptors. <i>Viruses</i> , <b>2018</b> , 10,   | 6.2  | 19 |
| 103 | Towards good correlation between fragment molecular orbital interaction energies and experimental IC for ligand binding: A case study of p38 MAP kinase. <i>Computational and Structural Biotechnology Journal</i> , <b>2018</b> , 16, 421-434  | 6.8  | 17 |
| 102 | Improved equation of state for finite-temperature spin-polarized electron liquids on the basis of Singwi-Tosi-LandSjlander approximation. <i>Contributions To Plasma Physics</i> , <b>2017</b> , 57, 126-136  | 1.4  | 11 |
| 101 | Meteorite impacts on ancient oceans opened up multiple NH production pathways. <i>Physical Chemistry Chemical Physics</i> , <b>2017</b> , 19, 11655-11667   | 3.6  | 2  |
| 100 | Cosolvent-Based Molecular Dynamics for Ensemble Docking: Practical Method for Generating Druggable Protein Conformations. <i>Journal of Chemical Information and Modeling</i> , <b>2017</b> , 57, 742-756   | 6.1  | 21 |
| 99  | Information geometrical characterization of the Onsager-Machlup process. <i>Chemical Physics Letters</i> , <b>2017</b> , 689, 152-155   | 2.5  | 2  |
| 98  | Structural transition of solvated H-Ras/GTP revealed by molecular dynamics simulation and local network entropy. <i>Journal of Molecular Graphics and Modelling</i> , <b>2017</b> , 77, 51-63   | 2.8  | 4  |
| 97  | Newly characterized interaction stabilizes DNA structure: oligoethylene glycols stabilize G-quadruplexes CH $\pi$ interactions. <i>Nucleic Acids Research</i> , <b>2017</b> , 45, 7021-7030   | 20.1 | 16 |
| 96  | Current Status of ABINIT-MP as a FMO Program and Related Works with Machine Learning. <i>Journal of Computer Chemistry Japan</i> , <b>2017</b> , 16, 119-122  | 0.2  | 6  |
| 95  | Theoretical Analysis of Activity Cliffs among Benzofuranone-Class Pim1 Inhibitors Using the Fragment Molecular Orbital Method with Molecular Mechanics Poisson-Boltzmann Surface Area (FMO+MM-PBSA) Approach. <i>Journal of Chemical Information and Modeling</i> , <b>2017</b> , 57, 2996-3010 | 6.1  | 25 |
| 94  | Local thermodynamics of the water molecules around single- and double-stranded DNA studied by grid inhomogeneous solvation theory. <i>Chemical Physics Letters</i> , <b>2016</b> , 660, 250-255   | 2.5  | 9  |
| 93  | Reduced minimum model for the photosynthetic induction processes in photosystem I. <i>Journal of Photochemistry and Photobiology B: Biology</i> , <b>2016</b> , 160, 364-75   | 6.7  | 4  |
| 92  | AutoDock-GIST: Incorporating Thermodynamics of Active-Site Water into Scoring Function for Accurate Protein-Ligand Docking. <i>Molecules</i> , <b>2016</b> , 21,  | 4.8  | 31 |
| 91  | Diffusion Monte Carlo study on temporal evolution of entropy and free energy in nonequilibrium processes. <i>Journal of Chemical Physics</i> , <b>2016</b> , 144, 094103  | 3.9  | 3  |

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| 90 | Meteorite Impact-Induced Rapid NH Production on Early Earth: Ab Initio Molecular Dynamics Simulation. <i>Scientific Reports</i> , <b>2016</b> , 6, 38953  | 4.9 | 12  |
| 89 | Correlational and thermodynamic properties of finite-temperature electron liquids in the hypernetted-chain approximation. <i>Journal of Chemical Physics</i> , <b>2016</b> , 145, 214104  | 3.9 | 21  |
| 88 | Four-electron model for singlet and triplet excitation energy transfers with inclusion of coherence memory, inelastic tunneling and nuclear quantum effects. <i>Chemical Physics</i> , <b>2016</b> , 474, 18-24   | 2.3 | 2   |
| 87 | Systems approach to excitation-energy and electron transfer reaction networks in photosystem II complex: model studies for chlorophyll a fluorescence induction kinetics. <i>Journal of Theoretical Biology</i> , <b>2015</b> , 380, 220-37   | 2.3 | 4   |
| 86 | Effects of Bridge Functions on Radial Distribution Functions of Liquid Water. <i>Interdisciplinary Sciences, Computational Life Sciences</i> , <b>2015</b> , 7, 152-6   | 3.5 |     |
| 85 | Protein-ligand docking using fitness learning-based artificial bee colony with proximity stimuli. <i>Physical Chemistry Chemical Physics</i> , <b>2015</b> , 17, 16412-7  | 3.6 | 18  |
| 84 | Novel type of virtual ligand screening on the basis of quantum-chemical calculations for protein-ligand complexes and extended clustering techniques. <i>Computational and Theoretical Chemistry</i> , <b>2015</b> , 1061, 12-22  | 2   | 18  |
| 83 | Thermodynamic properties of water molecules in the presence of cosolute depend on DNA structure: a study using grid inhomogeneous solvation theory. <i>Nucleic Acids Research</i> , <b>2015</b> , 43, 10114-25 <sup>20.1</sup>  |     | 22  |
| 82 | Explicit solvation modulates intra- and inter-molecular interactions within DNA: Electronic aspects revealed by the ab initio fragment molecular orbital (FMO) method. <i>Computational and Theoretical Chemistry</i> , <b>2015</b> , 1054, 29-37   | 2   | 16  |
| 81 | Theoretical prediction and experimental verification on enantioselectivity of haloacid dehalogenase I-DEX YL with chloropropionate. <i>Chemical Physics Letters</i> , <b>2015</b> , 623, 101-107  | 2.5 | 6   |
| 80 | Classical density functional calculation of radial distribution functions of liquid water. <i>Chemical Physics</i> , <b>2014</b> , 430, 18-22   | 2.3 | 3   |
| 79 | Electron-correlated fragment-molecular-orbital calculations for biomolecular and nano systems. <i>Physical Chemistry Chemical Physics</i> , <b>2014</b> , 16, 10310-44  | 3.6 | 200 |
| 78 | Charge clamps of lysines and hydrogen bonds play key roles in the mechanism to fix helix 12 in the agonist and antagonist positions of estrogen receptor. Intramolecular interactions studied by the ab initio fragment molecular orbital method. <i>Journal of Physical Chemistry B</i> , <b>2014</b> , 118, 4993-5008 | 3.4 | 18  |
| 77 | A significant role of Arg41 residue in the enzymatic reaction of haloacid dehalogenase I-DEX YL studied by QM/MM method. <i>Journal of Molecular Catalysis B: Enzymatic</i> , <b>2014</b> , 110, 23-31  |     | 8   |
| 76 | Interaction energy analysis on specific binding of influenza virus hemagglutinin to avian and human sialosaccharide receptors: importance of mutation-induced structural change. <i>Journal of Molecular Graphics and Modelling</i> , <b>2014</b> , 53, 48-58   | 2.8 | 16  |
| 75 | Affinity of molecular ions for DNA structures is determined by solvent-accessible surface area. <i>Journal of Physical Chemistry B</i> , <b>2014</b> , 118, 9583-94   | 3.4 | 16  |
| 74 | Hierarchical coarse-graining model for photosystem II including electron and excitation-energy transfer processes. <i>BioSystems</i> , <b>2014</b> , 117, 15-29   | 1.9 | 2   |
| 73 | Accuracy of the fragment molecular orbital (FMO) calculations for DNA: Total energy, molecular orbital, and inter-fragment interaction energy. <i>Computational and Theoretical Chemistry</i> , <b>2014</b> , 1034, 7-16  | 2   | 15  |

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| 72 | Study of the aggregation mechanism of polyglutamine peptides using replica exchange molecular dynamics simulations. <i>Journal of Molecular Modeling</i> , <b>2013</b> , 19, 1627-39   | 2   | 13 |
| 71 | Modeling of peptide-ligand interaction based on four-body corrected fragment molecular orbital (FMO4) calculations. <i>Chemical Physics Letters</i> , <b>2013</b> , 566, 25-31   | 2.5 | 27 |
| 70 | Statistical correction to effective interactions in the fragment molecular orbital method. <i>Chemical Physics Letters</i> , <b>2013</b> , 556, 272-277  | 2.5 | 36 |
| 69 | Triplet correlations and bridge functions in classical density functional theory for liquid water. <i>Chemical Physics Letters</i> , <b>2013</b> , 572, 38-43  | 2.5 | 3  |
| 68 | Three- and four-body corrected fragment molecular orbital calculations with a novel subdividing fragmentation method applicable to structure-based drug design. <i>Journal of Molecular Graphics and Modelling</i> , <b>2013</b> , 41, 31-42 | 2.8 | 41 |
| 67 | Variational Quantum Monte Carlo with Inclusion of Orbital Correlations. <i>Journal of the Physical Society of Japan</i> , <b>2013</b> , 82, 075001   | 1.5 | 2  |
| 66 | Development of the four-body corrected fragment molecular orbital (FMO4) method. <i>Chemical Physics Letters</i> , <b>2012</b> , 523, 128-133  | 2.5 | 52 |
| 65 | Ab initio path integral Monte Carlo simulations for water trimer with electron correlation effects. <i>Computational and Theoretical Chemistry</i> , <b>2012</b> , 997, 7-13   | 2   | 9  |
| 64 | Excitation energy transfer modulated by oscillating electronic coupling of a dimeric system embedded in a molecular environment. <i>Physical Review E</i> , <b>2012</b> , 86, 021914   | 2.4 | 3  |
| 63 | Renormalization-Group Inspired Approach to Vibrational Energy Transfer in Protein. <i>Journal of the Physical Society of Japan</i> , <b>2012</b> , 81, 033801  | 1.5 | 1  |
| 62 | Prediction of probable mutations in influenza virus hemagglutinin protein based on large-scale ab initio fragment molecular orbital calculations. <i>Journal of Molecular Graphics and Modelling</i> , <b>2011</b> , 30, 110-9               | 2.8 | 26 |
| 61 | Higher-order correlated calculations based on fragment molecular orbital scheme. <i>Theoretical Chemistry Accounts</i> , <b>2011</b> , 130, 515-530  | 1.9 | 64 |
| 60 | Antigen-Antibody interactions of influenza virus hemagglutinin revealed by the fragment molecular orbital calculation. <i>Theoretical Chemistry Accounts</i> , <b>2011</b> , 130, 1197-1202  | 1.9 | 16 |
| 59 | Fragment molecular orbital calculations under periodic boundary condition. <i>Chemical Physics Letters</i> , <b>2011</b> , 506, 112-116  | 2.5 | 35 |
| 58 | Modulation of excitation energy transfer by conformational oscillations in biomolecular systems. <i>Chemical Physics Letters</i> , <b>2011</b> , 508, 139-143  | 2.5 | 8  |
| 57 | Counterpoise-corrected interaction energy analysis based on the fragment molecular orbital scheme. <i>Chemical Physics Letters</i> , <b>2011</b> , 509, 67-71  | 2.5 | 22 |
| 56 | Sialic acid recognition of the pandemic influenza 2009 H1N1 virus: binding mechanism between human receptor and influenza hemagglutinin. <i>Protein and Peptide Letters</i> , <b>2011</b> , 18, 530-9  | 1.9 | 12 |
| 55 | Analysis of electron-transfer rate constant in condensed media with inclusion of inelastic tunneling and nuclear quantum effects. <i>Physical Review E</i> , <b>2010</b> , 81, 027101  | 2.4 | 8  |

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| 54 | Comparative characterization of short monomeric polyglutamine peptides by replica exchange molecular dynamics simulation. <i>Journal of Physical Chemistry B</i> , <b>2010</b> , 114, 7056-61  | 3.4 | 17 |
| 53 | Acceleration of fragment molecular orbital calculations with Cholesky decomposition approach. <i>Chemical Physics Letters</i> , <b>2010</b> , 490, 84-89   | 2.5 | 46 |
| 52 | Incorporation of solvation effects into the fragment molecular orbital calculations with the Poisson-Boltzmann equation. <i>Chemical Physics Letters</i> , <b>2010</b> , 500, 116-119  | 2.5 | 45 |
| 51 | Molecular mechanics and all-electron fragment molecular orbital calculations on mutated polyglutamine peptides. <i>Computational and Theoretical Chemistry</i> , <b>2010</b> , 944, 12-20  |     | 8  |
| 50 | Fragment molecular orbital (FMO) study on stabilization mechanism of neuro-oncological ventral antigen (NOVA) RNA complex system. <i>Computational and Theoretical Chemistry</i> , <b>2010</b> , 962, 45-55  |     | 16 |
| 49 | Large-scale FMO-MP3 calculations on the surface proteins of influenza virus, hemagglutinin (HA) and neuraminidase (NA). <i>Chemical Physics Letters</i> , <b>2010</b> , 493, 346-352   | 2.5 | 42 |
| 48 | Comparison of binding affinity evaluations for FKBP ligands with state-of-the-art computational methods: FMO, QM/MM, MM-PB/SA and MP-CAFE approaches. <i>Chem-Bio Informatics Journal</i> , <b>2010</b> , 10, 32-45  | 0.8 | 9  |
| 47 | Ab initio Path Integral Molecular Dynamics Based on Fragment Molecular Orbital Method. <i>Journal of the Physical Society of Japan</i> , <b>2009</b> , 78, 104723  | 1.5 | 20 |
| 46 | Roles of K151 and D180 in L-2-haloacid dehalogenase from <i>Pseudomonas</i> sp. YL: analysis by molecular dynamics and ab initio fragment molecular orbital calculations. <i>Journal of Computational Chemistry</i> , <b>2009</b> , 30, 2625-34  | 3.5 | 24 |
| 45 | Application of the fragment molecular orbital method for determination of atomic charges on polypeptides. II. Towards an improvement of force fields used for classical molecular dynamics simulations. <i>Chemical Physics Letters</i> , <b>2009</b> , 467, 417-423                           | 2.5 | 32 |
| 44 | Ab initio quantum-chemical study on emission spectra of bioluminescent luciferases by fragment molecular orbital method. <i>Chemical Physics Letters</i> , <b>2009</b> , 472, 118-123  | 2.5 | 36 |
| 43 | Accuracy of fragmentation in ab initio calculations of hydrated sodium cation. <i>Chemical Physics Letters</i> , <b>2009</b> , 478, 295-300  | 2.5 | 38 |
| 42 | Possibility of mutation prediction of influenza hemagglutinin by combination of hemadsorption experiment and quantum chemical calculation for antibody binding. <i>Journal of Physical Chemistry B</i> , <b>2009</b> , 113, 4991-4   | 3.4 | 45 |
| 41 | Fragment molecular orbital calculations on red fluorescent proteins (DsRed and mFruits). <i>Journal of Physical Chemistry B</i> , <b>2009</b> , 113, 1153-61   | 3.4 | 36 |
| 40 | Fragment Molecular Orbital (FMO) and FMO-MO Calculations of DNA: Accuracy Validation of Energy and Interfragment Interaction Energy. <i>Journal of Computational and Theoretical Nanoscience</i> , <b>2009</b> , 6, 1328-1337  | 0.3 | 21 |
| 39 | 1P-100 Study of RNA base recognition mechanism by aliphatic surface of RNA-binding protein : Case study of NOVA-RNA complex system(Nucleic acid:Interaction & Complex formation, The 47th Annual Meeting of the Biophysical Society of Japan). <i>Seibutsu Butsuri</i> , <b>2009</b> , 49, S79 | 0   |    |
| 38 | Application of the FMO Method to Specific Molecular Recognition of Biomacromolecules <b>2009</b> , 133-170   |     | 3  |
| 37 | 1TP5-05 Study of RNA base recognition mechanism by aliphatic surface of RNA-binding protein : Case study of NOVA-RNA complex system(The 47th Annual Meeting of the Biophysical Society of Japan). <i>Seibutsu Butsuri</i> , <b>2009</b> , 49, S37-S38  | 0   |    |

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| 36 | Ab initio fragment molecular orbital study of molecular interactions in liganded retinoid X receptor: specification of residues associated with ligand inducible information transmission. <i>Journal of Physical Chemistry B</i> , <b>2008</b> , 112, 12081-94   | 3.4 | 46  |
| 35 | 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. <i>Journal of Physical Chemistry A</i> , <b>2008</b> , 112, 1986-98 | 2.8 | 37  |
| 34 | Derivation of extremely slow dynamics of protein motion based on entropy invariance. <i>Physics Letters, Section A: General, Atomic and Solid State Physics</i> , <b>2008</b> , 372, 1280-1282  | 2.3 | 3   |
| 33 | Theoretical analysis of binding specificity of influenza viral hemagglutinin to avian and human receptors based on the fragment molecular orbital method. <i>Computational Biology and Chemistry</i> , <b>2008</b> , 32, 198-211  | 3.6 | 47  |
| 32 | Large scale FMO-MP2 calculations on a massively parallel-vector computer. <i>Chemical Physics Letters</i> , <b>2008</b> , 457, 396-403  | 2.5 | 100 |
| 31 | An application of fragment interaction analysis based on local MP2. <i>Chemical Physics Letters</i> , <b>2008</b> , 463, 189-194  | 2.5 | 27  |
| 30 | DNA and estrogen receptor interaction revealed by fragment molecular orbital calculations. <i>Journal of Physical Chemistry B</i> , <b>2007</b> , 111, 9621-7   | 3.4 | 40  |
| 29 | Fragment molecular orbital calculations on red fluorescent protein (DsRed). <i>Chemical Physics Letters</i> , <b>2007</b> , 433, 360-367  | 2.5 | 31  |
| 28 | Effects of salt addition on strength and dynamics of hydrophobic interactions. <i>Chemical Physics Letters</i> , <b>2007</b> , 434, 42-48   | 2.5 | 19  |
| 27 | Application of the fragment molecular orbital method for determination of atomic charges on polypeptides. <i>Chemical Physics Letters</i> , <b>2007</b> , 449, 329-335  | 2.5 | 28  |
| 26 | Visualization analysis of inter-fragment interaction energies of CRP-cAMP-DNA complex based on the fragment molecular orbital method. <i>Biophysical Chemistry</i> , <b>2007</b> , 130, 1-9   | 3.5 | 41  |
| 25 | Fragment interaction analysis based on local MP2. <i>Theoretical Chemistry Accounts</i> , <b>2007</b> , 118, 937-945  | 1.9 | 57  |
| 24 | Fragmentation Method Combined with Quantum Monte Carlo Calculations. <i>Journal of the Physical Society of Japan</i> , <b>2007</b> , 76, 064301   | 1.5 | 15  |
| 23 | Ab initio study of molecular interactions in higher plant and <i>Galdieria partita</i> Rubiscos with the fragment molecular orbital method. <i>Biochemical and Biophysical Research Communications</i> , <b>2007</b> , 361, 367-72  | 3.4 | 8   |
| 22 | Ab initio fragment molecular orbital study of molecular interactions between liganded retinoid X receptor and its coactivator: roles of helix 12 in the coactivator binding mechanism. <i>Journal of Physical Chemistry B</i> , <b>2007</b> , 111, 3525-33  | 3.4 | 32  |
| 21 | Intra- and intermolecular interactions between cyclic-AMP receptor protein and DNA: ab initio fragment molecular orbital study. <i>Journal of Computational Chemistry</i> , <b>2006</b> , 27, 948-60  | 3.5 | 97  |
| 20 | Molecular interactions between estrogen receptor and its ligand studied by the ab initio fragment molecular orbital method. <i>Journal of Physical Chemistry B</i> , <b>2006</b> , 110, 16102-10  | 3.4 | 106 |
| 19 | Dynamic polarizability calculation with fragment molecular orbital scheme. <i>Chemical Physics Letters</i> , <b>2006</b> , 418, 418-422   | 2.5 | 27  |



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|----|---|-----|----|
| 18 | Fragment molecular orbital calculations on large scale systems containing heavy metal atom. <i>Chemical Physics Letters</i> , <b>2006</b> , 427, 159-165  | 2.5 | 48 |
| 17 | Application of fragment molecular orbital scheme to silicon-containing systems. <i>Chemical Physics Letters</i> , <b>2006</b> , 430, 361-366  | 2.5 | 15 |
| 16 | Developments and applications of ABINIT-MP software based on the fragment molecular orbital method <b>2006</b> , 39-52  |     | 33 |
| 15 | A configuration analysis for fragment interaction. <i>Chemical Physics Letters</i> , <b>2005</b> , 410, 247-253   | 2.5 | 84 |
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