# Shigenori Tanaka

## List of Publications by Citations



| | | | |
|---|---|---|---|
| 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 | Electron-correlated fragment-molecular-orbital calculations for biomolecular and nano systems. *Physical Chemistry Chemical Physics*, **2014**, 16, 10310-44 | 3.6 | 200 |
| 142 | Molecular interactions between estrogen receptor and its ligand studied by the ab initio fragment molecular orbital method. *Journal of Physical Chemistry B*, **2006**, 110, 16102-10 | 3.4 | 106 |
| 141 | Large scale FMO-MP2 calculations on a massively parallel-vector computer. *Chemical Physics Letters* , **2008**, 457, 396-403 | 2.5 | 100 |
| 140 | Intra- and intermolecular interactions between cyclic-AMP receptor protein and DNA: ab initio fragment molecular orbital study. *Journal of Computational Chemistry*, **2006**, 27, 948-60 | 3.5 | 97 |
| 139 | Thermodynamics and Correlational Properties of Finite-Temperature Electron Liquids in the Singwi-Tosi-Land-Sjölander Approximation. *Journal of the Physical Society of Japan*, **1986**, 55, 2278-2289 | 1.5 | 90 |
| 138 | A configuration analysis for fragment interaction. *Chemical Physics Letters*, **2005**, 410, 247-253 | 2.5 | 84 |
| 137 | Generalized viscoelastic theory of the glass transition for strongly coupled, classical, one-component plasmas. *Physical Review Letters*, **1986**, 56, 2815-2818 | 7.4 | 73 |
| 136 | Higher-order correlated calculations based on fragment molecular orbital scheme. *Theoretical Chemistry Accounts*, **2011**, 130, 515-530 | 1.9 | 64 |
| 135 | Fragment interaction analysis based on local MP2. *Theoretical Chemistry Accounts*, **2007**, 118, 937-945 | 1.9 | 57 |
| 134 | Development of the four-body corrected fragment molecular orbital (FMO4) method. *Chemical Physics Letters*, **2012**, 523, 128-133 | 2.5 | 52 |
| 133 | Fragment Molecular Orbital Based Interaction Analyses on COVID-19 Main Protease - Inhibitor N3 Complex (PDB ID: 6LU7). *Journal of Chemical Information and Modeling*, **2020**, 60, 3593-3602 | 6.1 | 50 |
| 132 | Fragment molecular orbital calculations on large scale systems containing heavy metal atom. *Chemical Physics Letters*, **2006**, 427, 159-165 | 2.5 | 48 |
| 131 | Spin-dependent correlations and thermodynamic functions for electron liquids at arbitrary degeneracy and spin polarization. *Physical Review B*, **1989**, 39, 1036-1051 | 3.3 | 48 |
| 130 | Parametrized equation of state for electron liquids in the Singwi-Tosi-Land-Sjölander approximation. *Physical Review A*, **1985**, 32, 1896-1899 | 2.6 | 48 |
| 129 | Theoretical analysis of binding specificity of influenza viral hemagglutinin to avian and human receptors based on the fragment molecular orbital method. *Computational Biology and Chemistry*, **2008**, 32, 198-211 | 3.6 | 47 |
| 128 | Acceleration of fragment molecular orbital calculations with Cholesky decomposition approach. *Chemical Physics Letters*, **2010**, 490, 84-89 | 2.5 | 46 |
| 127 | Ab initio fragment molecular orbital study of molecular interactions in liganded retinoid X receptor: specification of residues associated with ligand inducible information transmission. *Journal of Physical Chemistry B*, **2008**, 112, 12081-94 | 3.4 | 46 |

| | | | |
|---|---|---|---|
| 126 | Possibility of mutation prediction of influenza hemagglutinin by combination of hemadsorption experiment and quantum chemical calculation for antibody binding. *Journal of Physical Chemistry B*, **2009**, 113, 4991-4 | 3.4 | 45 |
| 125 | Incorporation of solvation effects into the fragment molecular orbital calculations with the PoissonBoltzmann equation. *Chemical Physics Letters*, **2010**, 500, 116-119 | 2.5 | 45 |
| 124 | Large-scale FMO-MP3 calculations on the surface proteins of influenza virus, hemagglutinin (HA) and neuraminidase (NA). *Chemical Physics Letters*, **2010**, 493, 346-352 | 2.5 | 42 |
| 123 | Three- and four-body corrected fragment molecular orbital calculations with a novel subdividing fragmentation method applicable to structure-based drug design. *Journal of Molecular Graphics and Modelling*, **2013**, 41, 31-42 | 2.8 | 41 |
| 122 | Visualization analysis of inter-fragment interaction energies of CRP-cAMP-DNA complex based on the fragment molecular orbital method. *Biophysical Chemistry*, **2007**, 130, 1-9 | 3.5 | 41 |
| 121 | Dynamic theory of correlations in strongly coupled, classical one-component plasmas: Glass transition in the generalized viscoelastic formalism. *Physical Review A*, **1987**, 35, 4743-4754 | 2.6 | 41 |
| 120 | DNA and estrogen receptor interaction revealed by fragment molecular orbital calculations. *Journal of Physical Chemistry B*, **2007**, 111, 9621-7 | 3.4 | 40 |
| 119 | Accuracy of fragmentation in ab initio calculations of hydrated sodium cation. *Chemical Physics Letters*, **2009**, 478, 295-300 | 2.5 | 38 |
| 118 | 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. *Journal of Physical Chemistry A*, **2008**, 112, 1986-98 | 2.8 | 37 |
| 117 | Statistical correction to effective interactions in the fragment molecular orbital method. *Chemical Physics Letters*, **2013**, 556, 272-277 | 2.5 | 36 |
| 116 | Ab initio quantum-chemical study on emission spectra of bioluminescent luciferases by fragment molecular orbital method. *Chemical Physics Letters*, **2009**, 472, 118-123 | 2.5 | 36 |
| 115 | Fragment molecular orbital calculations on red fluorescent proteins (DsRed and mFruits). *Journal of Physical Chemistry B*, **2009**, 113, 1153-61 | 3.4 | 36 |
| 114 | Electron Transfer Model for the Electric Field Effect on Quantum Yield of Charge Separation in Bacterial Photosynthetic Reaction Centers. *Journal of Physical Chemistry B*, **1997**, 101, 5031-5045 | 3.4 | 36 |
| 113 | Fragment molecular orbital calculations under periodic boundary condition. *Chemical Physics Letters*, **2011**, 506, 112-116 | 2.5 | 35 |
| 112 | Fragment Molecular Orbital Calculations with Implicit Solvent Based on the Poisson-Boltzmann Equation: II. Protein and Its Ligand-Binding System Studies. *Journal of Physical Chemistry B*, **2019**, 123, 957-973 | 3.4 | 34 |
| 111 | Developments and applications of ABINIT-MP software based on the fragment molecular orbital method **2006**, 39-52 | | 33 |
| 110 | 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. *Chemical Physics Letters*, **2009**, 467, 417-423 | 2.5 | 32 |
| 109 | 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. *Journal of Physical Chemistry B*, **2007**, 111, 3525-33 | 3.4 | 32 |

| | | | |
|---|---|---|---|
| 108 | Fragment molecular orbital calculations on red fluorescent protein (DsRed). *Chemical Physics Letters*, **2007**, 433, 360-367 | 2.5 | 31 |
| 107 | AutoDock-GIST: Incorporating Thermodynamics of Active-Site Water into Scoring Function for Accurate Protein-Ligand Docking. *Molecules*, **2016**, 21, | 4.8 | 31 |
| 106 | Fragment Molecular Orbital Calculations with Implicit Solvent Based on the Poisson-Boltzmann Equation: Implementation and DNA Study. *Journal of Physical Chemistry B*, **2018**, 122, 4457-4471 | 3.4 | 28 |
| 105 | Application of the fragment molecular orbital method for determination of atomic charges on polypeptides. *Chemical Physics Letters*, **2007**, 449, 329-335 | 2.5 | 28 |
| 104 | Modeling of peptide–silica interaction based on four-body corrected fragment molecular orbital (FMO4) calculations. *Chemical Physics Letters*, **2013**, 566, 25-31 | 2.5 | 27 |
| 103 | An application of fragment interaction analysis based on local MP2. *Chemical Physics Letters*, **2008**, 463, 189-194 | 2.5 | 27 |
| 102 | Dynamic polarizability calculation with fragment molecular orbital scheme. *Chemical Physics Letters*, **2006**, 418, 418-422 | 2.5 | 27 |
| 101 | Prediction of probable mutations in influenza virus hemagglutinin protein based on large-scale ab initio fragment molecular orbital calculations. *Journal of Molecular Graphics and Modelling*, **2011**, 30, 110-9 | 2.8 | 26 |
| 100 | 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. *Journal of Chemical Information and Modeling*, **2017**, 57, 2996-3010 | 6.1 | 25 |
| 99 | Roles of K151 and D180 in L-2-haloacid dehalogenase from Pseudomonas sp. YL: analysis by molecular dynamics and ab initio fragment molecular orbital calculations. *Journal of Computational Chemistry*, **2009**, 30, 2625-34 | 3.5 | 24 |
| 98 | Effective Static Approximation: A Fast and Reliable Tool for Warm-Dense Matter Theory. *Physical Review Letters*, **2020**, 125, 235001 | 7.4 | 24 |
| 97 | Strongly coupled electron liquid: Ab initio path integral Monte Carlo simulations and dielectric theories. *Physical Review B*, **2020**, 101, | 3.3 | 22 |
| 96 | Thermodynamic properties of water molecules in the presence of cosolute depend on DNA structure: a study using grid inhomogeneous solvation theory. *Nucleic Acids Research*, **2015**, 43, 10114-25 | 20.1 | 22 |
| 95 | Counterpoise-corrected interaction energy analysis based on the fragment molecular orbital scheme. *Chemical Physics Letters*, **2011**, 509, 67-71 | 2.5 | 22 |
| 94 | Molecular recognition of SARS-CoV-2 spike glycoprotein: quantum chemical hot spot and epitope analyses.. *Chemical Science*, **2021**, 12, 4722-4739 | 9.4 | 22 |
| 93 | Cosolvent-Based Molecular Dynamics for Ensemble Docking: Practical Method for Generating Druggable Protein Conformations. *Journal of Chemical Information and Modeling*, **2017**, 57, 742-756 | 6.1 | 21 |
| 92 | Fragment Molecular Orbital (FMO) and FMO-MO Calculations of DNA: Accuracy Validation of Energy and Interfragment Interaction Energy. *Journal of Computational and Theoretical Nanoscience* , **2009**, 6, 1328-1337 | 0.3 | 21 |
| 91 | Correlational and thermodynamic properties of finite-temperature electron liquids in the hypernetted-chain approximation. *Journal of Chemical Physics*, **2016**, 145, 214104 | 3.9 | 21 |

| | | | |
|---|---|---|---|
| 90 | Ab initioPath Integral Molecular Dynamics Based on Fragment Molecular Orbital Method. *Journal of the Physical Society of Japan*, **2009**, 78, 104723 | 1.5 | 20 |
| 89 | Nuclear quantum effects on electron transfer reactions in DNA hairpins. *Physical Review E*, **2003**, 68, 031905 | 2.4 | 20 |
| 88 | DENSITY FUNCTIONAL CALCULATIONS ON THE INTERACTION BETWEEN CATABOLITE ACTIVATOR PROTEIN AND CYCLIC AMP USING THE FRAGMENT MOLECULAR ORBITAL METHOD. *Journal of Theoretical and Computational Chemistry*, **2005**, 04, 183-195 | 1.8 | 20 |
| 87 | Ion-Density Correlations and Enhancement of Thermonuclear Reaction Rate in Dense, Inertially Confined Fusion Plasmas. *Journal of the Physical Society of Japan*, **1984**, 53, 2039-2048 | 1.5 | 20 |
| 86 | Stopping Power of Degenerate Electron Liquid at Metallic Densities. *Journal of the Physical Society of Japan*, **1985**, 54, 2537-2542 | 1.5 | 20 |
| 85 | Computational Analysis of the Interaction Energies between Amino Acid Residues of the Measles Virus Hemagglutinin and Its Receptors. *Viruses*, **2018**, 10, | 6.2 | 19 |
| 84 | Effects of salt addition on strength and dynamics of hydrophobic interactions. *Chemical Physics Letters*, **2007**, 434, 42-48 | 2.5 | 19 |
| 83 | Theory of interparticle correlations in dense, high-temperature plasmas. VIII. Shear viscosity. *Physical Review A*, **1986**, 34, 4163-4170 | 2.6 | 19 |
| 82 | Protein-ligand docking using fitness learning-based artificial bee colony with proximity stimuli. *Physical Chemistry Chemical Physics*, **2015**, 17, 16412-7 | 3.6 | 18 |
| 81 | Novel type of virtual ligand screening on the basis of quantum-chemical calculations for protein□gand complexes and extended clustering techniques. *Computational and Theoretical Chemistry*, **2015**, 1061, 12-22 | 2 | 18 |
| 80 | Development of an automated fragment molecular orbital (FMO) calculation protocol toward construction of quantum mechanical calculation database for large biomolecules . *Chem-Bio Informatics Journal*, **2019**, 19, 5-18 | 0.8 | 18 |
| 79 | 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. *Journal of Physical Chemistry B*, **2014**, 118, 4993-5008 | 3.4 | 18 |
| 78 | Application of singular value decomposition to the inter-fragment interaction energy analysis for ligand screening. *Computational and Theoretical Chemistry*, **2018**, 1132, 23-34 | 2 | 17 |
| 77 | Comparative characterization of short monomeric polyglutamine peptides by replica exchange molecular dynamics simulation. *Journal of Physical Chemistry B*, **2010**, 114, 7056-61 | 3.4 | 17 |
| 76 | Towards good correlation between fragment molecular orbital interaction energies and experimental IC for ligand binding: A case study of p38 MAP kinase. *Computational and Structural Biotechnology Journal*, **2018**, 16, 421-434 | 6.8 | 17 |
| 75 | Interaction energy analysis on specific binding of influenza virus hemagglutinin to avian and human sialosaccharide receptors: importance of mutation-induced structural change. *Journal of Molecular Graphics and Modelling*, **2014**, 53, 48-58 | 2.8 | 16 |
| 74 | Affinity of molecular ions for DNA structures is determined by solvent-accessible surface area. *Journal of Physical Chemistry B*, **2014**, 118, 9583-94 | 3.4 | 16 |
| 73 | Newly characterized interaction stabilizes DNA structure: oligoethylene glycols stabilize G-quadruplexes CH-□interactions. *Nucleic Acids Research*, **2017**, 45, 7021-7030 | 20.1 | 16 |

| | | | |
|---|---|---|---|
| 72 | Explicit solvation modulates intra- and inter-molecular interactions within DNA: Electronic aspects revealed by the ab initio fragment molecular orbital (FMO) method. *Computational and Theoretical Chemistry*, **2015**, 1054, 29-37 | 2 | 16 |
| 71 | Antigen–antibody interactions of influenza virus hemagglutinin revealed by the fragment molecular orbital calculation. *Theoretical Chemistry Accounts*, **2011**, 130, 1197-1202 | 1.9 | 16 |
| 70 | Fragment molecular orbital (FMO) study on stabilization mechanism of neuro-oncological ventral antigen (NOVA)–RNA complex system. *Computational and Theoretical Chemistry*, **2010**, 962, 45-55 | | 16 |
| 69 | Accuracy of the fragment molecular orbital (FMO) calculations for DNA: Total energy, molecular orbital, and inter-fragment interaction energy. *Computational and Theoretical Chemistry*, **2014**, 1034, 7-16 | 2 | 15 |
| 68 | Fragmentation Method Combined with Quantum Monte Carlo Calculations. *Journal of the Physical Society of Japan*, **2007**, 76, 064301 | 1.5 | 15 |
| 67 | Application of fragment molecular orbital scheme to silicon-containing systems. *Chemical Physics Letters*, **2006**, 430, 361-366 | 2.5 | 15 |
| 66 | Theory of nonadiabatic electron transfer at electrode/liquid interfaces: Role of quantum effects. *Journal of Chemical Physics*, **1999**, 111, 11117-11137 | 3.9 | 14 |
| 65 | Study of the aggregation mechanism of polyglutamine peptides using replica exchange molecular dynamics simulations. *Journal of Molecular Modeling*, **2013**, 19, 1627-39 | 2 | 13 |
| 64 | Sialic acid recognition of the pandemic influenza 2009 H1N1 virus: binding mechanism between human receptor and influenza hemagglutinin. *Protein and Peptide Letters*, **2011**, 18, 530-9 | 1.9 | 12 |
| 63 | Meteorite Impact-Induced Rapid NH Production on Early Earth: Ab Initio Molecular Dynamics Simulation. *Scientific Reports*, **2016**, 6, 38953 | 4.9 | 12 |
| 62 | Improved equation of state for finite-temperature spin-polarized electron liquids on the basis of Singwi–Tosi–Land–Sjölander approximation. *Contributions To Plasma Physics*, **2017**, 57, 126-136 | 1.4 | 11 |
| 61 | Identification of correlated inter-residue interactions in protein complex based on the fragment molecular orbital method. *Journal of Molecular Graphics and Modelling*, **2020**, 100, 107650 | 2.8 | 11 |
| 60 | FMODB: The World's First Database of Quantum Mechanical Calculations for Biomacromolecules Based on the Fragment Molecular Orbital Method. *Journal of Chemical Information and Modeling*, **2021**, 61, 777-794 | 6.1 | 11 |
| 59 | Interaction analyses of SARS-CoV-2 spike protein based on fragment molecular orbital calculations.. *RSC Advances*, **2021**, 11, 3272-3279 | 3.7 | 11 |
| 58 | Statistical interaction analyses between SARS-CoV-2 main protease and inhibitor N3 by combining molecular dynamics simulation and fragment molecular orbital calculation. *Applied Physics Express*, **2021**, 14, 027003 | 2.4 | 10 |
| 57 | Local thermodynamics of the water molecules around single- and double-stranded DNA studied by grid inhomogeneous solvation theory. *Chemical Physics Letters*, **2016**, 660, 250-255 | 2.5 | 9 |
| 56 | Ab initio path integral Monte Carlo simulations for water trimer with electron correlation effects. *Computational and Theoretical Chemistry*, **2012**, 997, 7-13 | 2 | 9 |
| 55 | Comparison of binding affinity evaluations for FKBP ligands with state-of-the-art computational methods: FMO, QM/MM, MM-PB/SA and MP-CAFEE approaches. *Chem-Bio Informatics Journal*, **2010**, 10, 32-45 | 0.8 | 9 |

| | | | |
|---|---|---|---|
| 54 | ATP Converts A□Oligomer into Off-Pathway Species by Making Contact with Its Backbone Atoms Using Hydrophobic Adenosine. *Journal of Physical Chemistry B*, **2019**, 123, 9922-9933 | 3.4 | 9 |
| 53 | A significant role of Arg41 residue in the enzymatic reaction of haloacid dehalogenase l-DEX YL studied by QM/MM method. *Journal of Molecular Catalysis B: Enzymatic*, **2014**, 110, 23-31 | | 8 |
| 52 | Analysis of electron-transfer rate constant in condensed media with inclusion of inelastic tunneling and nuclear quantum effects. *Physical Review E*, **2010**, 81, 027101 | 2.4 | 8 |
| 51 | Modulation of excitation energy transfer by conformational oscillations in biomolecular systems. *Chemical Physics Letters*, **2011**, 508, 139-143 | 2.5 | 8 |
| 50 | Molecular mechanics and all-electron fragment molecular orbital calculations on mutated polyglutamine peptides. *Computational and Theoretical Chemistry*, **2010**, 944, 12-20 | | 8 |
| 49 | Ab initio study of molecular interactions in higher plant and Galdieria partita Rubiscos with the fragment molecular orbital method. *Biochemical and Biophysical Research Communications*, **2007**, 361, 367-72 | 3.4 | 8 |
| 48 | Dynamic Cooperativity of Ligand-Residue Interactions Evaluated with the Fragment Molecular Orbital Method. *Journal of Physical Chemistry B*, **2021**, 125, 6501-6512 | 3.4 | 8 |
| 47 | Statistical-Mechanical Theory of Cold Nuclear Fusion in Metal Hydrides. *Journal of the Physical Society of Japan*, **1990**, 59, 1333-1340 | 1.5 | 7 |
| 46 | Current Status of ABINIT-MP as a FMO Program and Related Works with Machine Learning. *Journal of Computer Chemistry Japan*, **2017**, 16, 119-122 | 0.2 | 6 |
| 45 | Theoretical prediction and experimental verification on enantioselectivity of haloacid dehalogenase l-DEX YL with chloropropionate. *Chemical Physics Letters*, **2015**, 623, 101-107 | 2.5 | 6 |
| 44 | Taking Water into Account with the Fragment Molecular Orbital Method. *Methods in Molecular Biology*, **2020**, 2114, 105-122 | 1.4 | 6 |
| 43 | Systems approach to excitation-energy and electron transfer reaction networks in photosystem II complex: model studies for chlorophyll a fluorescence induction kinetics. *Journal of Theoretical Biology*, **2015**, 380, 220-37 | 2.3 | 4 |
| 42 | Reduced minimum model for the photosynthetic induction processes in photosystem I. *Journal of Photochemistry and Photobiology B: Biology*, **2016**, 160, 364-75 | 6.7 | 4 |
| 41 | Structural transition of solvated H-Ras/GTP revealed by molecular dynamics simulation and local network entropy. *Journal of Molecular Graphics and Modelling*, **2017**, 77, 51-63 | 2.8 | 4 |
| 40 | New Modified Deoxythymine with Dibranched Tetraethylene Glycol Stabilizes G-Quadruplex Structures. *Molecules*, **2020**, 25, | 4.8 | 3 |
| 39 | Classical density functional calculation of radial distribution functions of liquid water. *Chemical Physics*, **2014**, 430, 18-22 | 2.3 | 3 |
| 38 | Triplet correlations and bridge functions in classical density functional theory for liquid water. *Chemical Physics Letters*, **2013**, 572, 38-43 | 2.5 | 3 |
| 37 | Excitation energy transfer modulated by oscillating electronic coupling of a dimeric system embedded in a molecular environment. *Physical Review E*, **2012**, 86, 021914 | 2.4 | 3 |

| | | | |
|---|---|---|---|
| 36 | Derivation of extremely slow dynamics of protein motion based on entropy invariance. *Physics Letters, Section A: General, Atomic and Solid State Physics*, **2008**, 372, 1280-1282 | 2.3 | 3 |
| 35 | Application of the FMO Method to Specific Molecular Recognition of Biomacromolecules **2009**, 133-170 | | 3 |
| 34 | Fragment molecular orbital calculations for biomolecules. *Current Opinion in Structural Biology*, **2021**, 72, 127-134 | 8.1 | 3 |
| 33 | Comparative study on model parameter evaluations for the energy transfer dynamics in Fenna□Matthews□Olson complex. *Chemical Physics*, **2020**, 539, 110903 | 2.3 | 3 |
| 32 | Diffusion Monte Carlo study on temporal evolution of entropy and free energy in nonequilibrium processes. *Journal of Chemical Physics*, **2016**, 144, 094103 | 3.9 | 3 |
| 31 | Non-Equilibrium Quantum Brain Dynamics: Super-Radiance and Equilibration in 21 Dimensions+. *Entropy*, **2019**, 21, 1066 | 2.8 | 3 |
| 30 | Ab initio molecular dynamics study of prebiotic production processes of organic compounds at meteorite impacts on ocean. *Journal of Computational Chemistry*, **2019**, 40, 349-359 | 3.5 | 3 |
| 29 | Fragment molecular orbital based interaction analyses on complexes between SARS-CoV-2 RBD variants and ACE2. *Japanese Journal of Applied Physics*, **2021**, 60, 090901 | 1.4 | 3 |
| 28 | Meteorite impacts on ancient oceans opened up multiple NH production pathways. *Physical Chemistry Chemical Physics*, **2017**, 19, 11655-11667 | 3.6 | 2 |
| 27 | Information geometrical characterization of the Onsager-Machlup process. *Chemical Physics Letters* , **2017**, 689, 152-155 | 2.5 | 2 |
| 26 | Hierarchical coarse-graining model for photosystem II including electron and excitation-energy transfer processes. *BioSystems*, **2014**, 117, 15-29 | 1.9 | 2 |
| 25 | Variational Quantum Monte Carlo with Inclusion of Orbital Correlations. *Journal of the Physical Society of Japan*, **2013**, 82, 075001 | 1.5 | 2 |
| 24 | Collective residue interactions in trimer complexes of SARS-CoV-2 spike proteins analyzed by fragment molecular orbital method. *Applied Physics Express*, **2022**, 15, 017001 | 2.4 | 2 |
| 23 | Molecular Recognition of SARS-CoV-2 Spike Glycoprotein: Quantum Chemical Hot Spot and Epitope Analyses | | 2 |
| 22 | Machine learning prediction of inter-fragment interaction energies between ligand and amino-acid residues on the fragment molecular orbital calculations for Janus kinase □nhibitor complex. *Chemical Physics Letters*, **2020**, 757, 137883 | 2.5 | 2 |
| 21 | Non-equilibrium Quantum Brain Dynamics II: Formulation in 3+1 dimensions. *Physica A: Statistical Mechanics and Its Applications*, **2021**, 567, 125706 | 3.3 | 2 |
| 20 | Four-electron model for singlet and triplet excitation energy transfers with inclusion of coherence memory, inelastic tunneling and nuclear quantum effects. *Chemical Physics*, **2016**, 474, 18-24 | 2.3 | 2 |
| 19 | The ABINIT-MP Program **2021**, 53-67 | | 2 |

| | | | |
|---|---|---|---|
| 18 | Nanoscale Quantum Thermal Conductance at Water Interface: Green Function Approach Based on One-Dimensional Phonon Model. *Molecules*, **2020**, 25, | 4.8 | 1 |
| 17 | Renormalization-Group Inspired Approach to Vibrational Energy Transfer in Protein. *Journal of the Physical Society of Japan*, **2012**, 81, 033801 | 1.5 | 1 |
| 16 | Remarked Suppression of A Protomer-Protomer Dissociation Reaction Elucidated by Molecular Dynamics Simulation.. *Proteins: Structure, Function and Bioinformatics*, **2022**, | 4.2 | 1 |
| 15 | 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. *Physical Chemistry Chemical Physics*, **2021**, 23, 26151-26164 | 3.6 | 1 |
| 14 | Non-Equilibrium Quantum Electrodynamics in Open Systems as a Realizable Representation of Quantum Field Theory of the Brain. *Entropy*, **2019**, 22, | 2.8 | 1 |
| 13 | Nonequilibrium quantum brain dynamics. *Advances in Quantum Chemistry*, **2020**, 82, 159-180 | 1.4 | 1 |
| 12 | Appearance of Thermal Time. *Foundations of Physics*, **2021**, 51, | 1.2 | 1 |
| 11 | Reaction Pathway Sampling and Free-Energy Analyses for Multimeric Protein Complex Disassembly by Employing Hybrid Configuration Bias Monte Carlo/Molecular Dynamics Simulation. *ACS Omega*, **2021**, 6, 4749-4758 | 3.9 | 1 |
| 10 | FMO Drug Design Consortium **2021**, 127-181 | | 1 |
| 9 | Temperature relaxation in binary hard-sphere mixture system: Molecular dynamics and kinetic theory study. *Journal of Chemical Physics*, **2020**, 153, 034114 | 3.9 | 0 |
| 8 | Effects of Bridge Functions on Radial Distribution Functions of Liquid Water. *Interdisciplinary Sciences, Computational Life Sciences*, **2015**, 7, 152-6 | 3.5 | |
| 7 | 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). *Seibutsu Butsuri*, **2009**, 49, S79 | 0 | |
| 6 | 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). *Seibutsu Butsuri*, **2009**, 49, S37-S38 | 0 | |
| 5 | In silico modeling of PAX8-PPAR fusion protein in thyroid carcinoma: influence of structural perturbation by fusion on ligand-binding affinity. *Journal of Computer-Aided Molecular Design*, **2021**, 35, 629-642 | 4.2 | |
| 4 | Density-Matrix Based Scheme of Basis Selection for Linear Combination of Fragment Molecular Orbitals. *Journal of the Physical Society of Japan*, **2021**, 90, 064301 | 1.5 | |
| 3 | Comparison of Various Fragmentation Methods for Quantum Chemical Calculations of Large Molecular Systems **2021**, 15-27 | | |
| 2 | Fragment Molecular Orbital Method as Cluster Expansion **2021**, 3-14 | | |
| 1 | Quantum Brain Dynamics in 2+1 dimensions: Non-equilibrium analysis towards memory formations. *Physica A: Statistical Mechanics and Its Applications*, **2022**, 598, 127397 | 3.3 | |