Takeshi Yamamoto

List of Publications by Year
in descending order

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56 papers	2,495 citations	201575 27 h-index	189801 50 g-index
58 all docs	58 docs citations	58 times ranked	1722 citing authors

#	Article	IF	Citations
1	High-Molecular-Weight Polyquinoxaline-Based Helically Chiral Phosphine (PQXphos) as Chirality-Switchable, Reusable, and Highly Enantioselective Monodentate Ligand in Catalytic Asymmetric Hydrosilylation of Styrenes. Journal of the American Chemical Society, 2010, 132, 7899-7901.	6.6	244
2	Highly Enantioselective Synthesis of Axially Chiral Biarylphosphonates: Asymmetric Suzukiâ€“Miyaura Coupling Using Highâ€Molecularâ€Weight, Helically Chiral Polyquinoxalineâ€Based Phosphines. Angewandte Chemie - International Edition, 2011, 50, 8844-8847.	7.2	209
3	Helical Poly(quinoxalineâ€2,3â€diyl)s Bearing Metalâ€Binding Sites as Polymerâ€Based Chiral Ligands for Asymmetric Catalysis. Angewandte Chemie - International Edition, 2009, 48, 539-542.	7.2	174
4	Solvent-Dependent Switch of Helical Main-Chain Chirality in Sergeants-and-Soldiers-Type Poly(quinoxaline-2,3-diyl)s: Effect of the Position and Structures of the â€œSergeantâ€•Chiral Units on the Screw-Sense Induction. Journal of the American Chemical Society, 2013, 135, 10104-10113.	6.6	123
5	Enhanced Catalyst Activity and Enantioselectivity with Chirality-Switchable Polymer Ligand PQXphos in Pd-Catalyzed Asymmetric Silaborative Cleavage of meso-Methylenecyclopropanes. Journal of the American Chemical Society, 2012, 134, 11092-11095.	6.6	122
6	Path integral calculation of thermal rate constants within the quantum instanton approximation: Application to the H+CH4â†'H2+CH3 hydrogen abstraction reaction in full Cartesian space. Journal of Chemical Physics, 2004, 120, 3100-3107.	1.2	101
7	Single-Handed Helical Poly(quinoxaline-2,3-diyl)s Bearing Achiral 4-Aminopyrid-3-yl Pendants as Highly Enantioselective, Reusable Chiral Nucleophilic Organocatalysts in the Steglich Reaction. Journal of the American Chemical Society, 2017, 139, 2557-2560.	6.6	89
8	Catalytic asymmetric synthesis using chirality-switchable helical polymer as a chiral ligand. Pure and Applied Chemistry, 2012, 84, 1759-1769.	0.9	85
9	Combining semiclassical time evolution and quantum Boltzmann operator to evaluate reactive flux correlation function for thermal rate constants of complex systems. Journal of Chemical Physics, 2002, 116, 7335-7349.	1.2	79
10	Chiral Palladacycle Catalysts Generated on a Singleâ€Handed Helical Polymer Skeleton for Asymmetric Arylative Ring Opening of 1,4â€Epoxyâ€1,4â€dihydronaphthalene. Angewandte Chemie - International Edition, 2014, 53, 12785-12788.	7.2	78
11	On the efficient path integral evaluation of thermal rate constants within the quantum instanton approximation. Journal of Chemical Physics, 2004, 120, 3086-3099.	1.2	76
12	Path integral evaluation of the quantum instanton rate constant for proton transfer in a polar solvent. Journal of Chemical Physics, 2005, 122, 044106.	1.2	72
13	Chirality-Amplifying, Dynamic Induction of Single-Handed Helix by Chiral Guests to Macromolecular Chiral Catalysts Bearing Boronyl Pendants as Receptor Sites. Journal of the American Chemical Society, 2018, 140, 3867-3870.	6.6	61
14	Variational and perturbative formulations of quantum mechanical/molecular mechanical free energy with mean-field embedding and its analytical gradients. Journal of Chemical Physics, 2008, 129, 244104.	1.2	58
15	Variational calculation of quantum mechanical/molecular mechanical free energy with electronic polarization of solvent. Journal of Chemical Physics, 2012, 136, 134107.	1.2	52
16	Theoretical study of the dissociation reaction HFCOâ†'HF+CO: New ab initio potential function and classical trajectory analysis. Journal of Chemical Physics, 1997, 107, 6114-6122.	1.2	44
17	Proton Transfer Studied Using a Combined Ab Initio Reactive Potential Energy Surface with Quantum Path Integral Methodology. Journal of Chemical Theory and Computation, 2010, 6, 2566-2580.	2.3	44
18	Asymmetric Suzukiâ€“Miyaura cross-coupling of 1-bromo-2-naphthoates using the helically chiral polymer ligand PQXphos. Chemical Communications, 2015, 51, 7211-7214.	2.2	37

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19	Anthranilamide-masked o-Iodoarylboronic Acids as Coupling Modules for Iterative Synthesis of ortho-Linked Oligoarenes. Chemistry Letters, 2013, 42, 541-543.	0.7	35
20	A wave-function based approach for polarizable charge model: Systematic comparison of polarization effects on protic, aprotic, and ionic liquids. Journal of Chemical Physics, 2010, 132, 044106.	1.2	33
21	Accurate and Efficient Treatment of Continuous Solute Charge Density in the Mean-Field QM/MM Free Energy Calculation. Journal of Chemical Theory and Computation, 2013, 9, 188-203.	2.3	31
22	Chirality-Switchable 2,2â€²-Bipyridine Ligands Attached to Helical Poly(quinoxaline-2,3-diyl)s for Copper-Catalyzed Asymmetric Cyclopropanation of Alkenes. ACS Macro Letters, 2017, 6, 705-710.	2.3	31
23	Boryl-Directed, Ir-Catalyzed C(sp³)â€“H Borylation of Alkylboronic Acids Leading to Site-Selective Synthesis of Polyborylalkanes. Organic Letters, 2019, 21, 6235-6240.	2.4	31
24	Complementary Induction of Right- and Left-Handed Helical Structures by the Positioning of Chiral Groups on the Monomer Units: Introduction of (â^)-Menthol as Side Chains of Poly(quinoxaline-2,3-diyl)s. ACS Macro Letters, 2013, 2, 790-793.	2.3	28
25	Regioselective Synthesis of o-Benzenediboronic Acids via Ir-Catalyzed o-Câ€“H Borylation Directed by a Pyrazolylaniline-Modified Boronyl Group. Organic Letters, 2017, 19, 886-889.	2.4	28
26	Full-dimensional quantum dynamics study on the mode-specific unimolecular dissociation reaction of HFCO. Journal of Chemical Physics, 2000, 112, 8006-8016.	1.2	23
27	Enantioconvergent Cu-Catalyzed Intramolecular Câ€“C Coupling at Boron-Bound C(sp³) Atoms of Î±-Aminoalkylboronates Using a C₁-Symmetrical 2,2â€²-Bipyridyl Ligand Attached to a Helically Chiral Macromolecular Scaffold. Journal of the American Chemical Society, 2020, 142, 18317-18323.	6.6	23
28	Like-Charge Attraction of Molecular Cations in Water: Subtle Balance between Interionic Interactions and Ionic Solvation Effect. Journal of Physical Chemistry B, 2014, 118, 5499-5508.	1.2	22
29	Quantum dynamics of unimolecular dissociation reaction HFCOâ†'HF+CO. Journal of Chemical Physics, 1998, 109, 9783-9794.	1.2	19
30	High-Temperature Plasticity of the β-phase in Nearly-Equiatomic Nickel-Titanium Alloys. Materials Transactions, JIM, 1999, 40, 343-350.	0.9	18
31	Ab initio calculation of proton-coupled electron transfer rates using the external-potential representation: A ubiquinol complex in solution. Journal of Chemical Physics, 2007, 126, 224514.	1.2	18
32	Chiral Palladacycle Catalysts Generated on a Singleâ€Handed Helical Polymer Skeleton for Asymmetric Arylative Ring Opening of 1,4â€Epoxyâ€1,4â€dihydronaphthalene. Angewandte Chemie, 2014, 126, 12999-13002.	1.6	18
33	Câ€“H Activation-Based Transformation of Naphthalenes to 3-Iodo-2-naphthylboronic Acid Derivatives for Use in Iterative Coupling Synthesis of Helical Oligo(naphthalene-2,3-diyl)s. Bulletin of the Chemical Society of Japan, 2017, 90, 604-606.	2.0	16
34	Stereoinvertive Câ€“C Bond Formation at the Boronâ€Bound Stereogenic Centers through Copperâ€Bipyridineâ€Catalyzed Intramolecular Coupling of Î±â€Aminobenzylboronic Esters. Angewandte Chemie - International Edition, 2020, 59, 7251-7255.	7.2	16
35	Preferred dissociative mechanism of phosphate monoester hydrolysis in low dielectric environments. Chemical Physics Letters, 2010, 500, 263-266.	1.2	13
36	Protonâ€coupled electron transfer of the phenoxyl/phenol couple: Effect of Hartreeâ€Fock exchange on transition structures. Journal of Computational Chemistry, 2011, 32, 3081-3091.	1.5	13

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37	Assessing the accuracy of integral equation theories for nano-sized hydrophobic solutes in water. Journal of Chemical Physics, 2017, 147, 014110.	1.2	12
38	Relating stacking structures and charge transport in crystal polymorphs of the pyrrole-based Ï€-conjugated molecule. Organic Electronics, 2017, 49, 53-63.	1.4	11
39	Helical Poly(quinoxalineâ€2,3â€diyl)s Bearing 1,2,3â€Triazole Pendants: Synthesis by CuAAC and Use as Reusable Abnormal NHC Ligands in Gold Catalysis. ChemCatChem, 2019, 11, 424-429.	1.8	11
40	Path-integral virial estimator for reaction-rate calculation based on the quantum instanton approximation. Journal of Chemical Physics, 2006, 124, 084102.	1.2	10
41	Solution reaction space Hamiltonian based on an electrostatic potential representation of solvent dynamics. Journal of Chemical Physics, 2011, 134, 144108.	1.2	10
42	Communication: Self-assembly of a model supramolecular polymer studied by replica exchange with solute tempering. Journal of Chemical Physics, 2017, 147, 211102.	1.2	10
43	Asymmetric O-to-C Aryloxycarbonyl Migration of Indolyl Carbonates Using Single-Handed Dynamic Helical Polyquinoxalines Bearing 4-Aminopyridyl Groups as Chiral Nucleophilic Catalysts. Bulletin of the Chemical Society of Japan, 2021, 94, 943-949.	2.0	10
44	PQXdpap: Helical Poly(quinoxaline-2,3-diyl)s Bearing 4-(Dipropylamino)pyridin-3-yl Pendants as Chirality-Switchable Nucleophilic Catalysts for the Kinetic Resolution of Secondary Alcohols. Organic Letters, 2021, 23, 8711-8716.	2.4	8
45	Quantum Mechanical Reaction Probability of Triplet Ketene at the Multireference Second-Order Perturbation Level of Theory. Journal of Physical Chemistry A, 2010, 114, 9981-9990.	1.1	7
46	Ab Initio Trajectory Study on Triplet Ketene Photodissociation via Statistical Sampling of the Crossing Seam. Journal of Chemical Theory and Computation, 2011, 7, 2507-2519.	2.3	7
47	Rhodium-catalyzed C(sp²)â€“H Addition of Arylboronic Acids to Alkynes Using a Boron-based, Convertible ortho-Directing Group. Chemistry Letters, 2017, 46, 1169-1172.	0.7	7
48	Comment on â€œComment on â€˜Simple reversible molecular dynamics algorithms for NosÃ©-Hoover chain dynamicsâ€™â€‰â€•[J. Chem. Phys. 110, 3623 (1999)]. Journal of Chemical Physics, 2006, 124, 217101.	1.2	5
49	Including charge penetration effects into the ESP derived partial charge operator. Chemical Physics Letters, 2012, 546, 80-85.	1.2	5
50	Self-Assembly of Nanocubic Molecular Capsules via Solvent-Guided Formation of Rectangular Blocks. Journal of Physical Chemistry Letters, 2018, 9, 6082-6088.	2.1	5
51	Multireference coupled-cluster calculation of the dissociation energy profile of triplet ketene. Chemical Physics Letters, 2011, 511, 28-32.	1.2	4
52	Coarse-grained modeling of nanocube self-assembly system and transition network analyses. Chemical Physics Letters, 2020, 742, 137135.	1.2	4
53	Amphiphilic Immobilized Diphenylprolinol Alkyl Ether Catalyst on PS-PEG Resin. Bulletin of the Chemical Society of Japan, 2021, 94, 790-797.	2.0	3
54	Stereoinvertive Câ€“C Bond Formation at the Boronâ€Bound Stereogenic Centers through Copperâ€Bipyridineâ€Catalyzed Intramolecular Coupling of Î±â€Aminobenzylboronic Esters. Angewandte Chemie, 2020, 132, 7318-7322.	1.6	1

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55	Connection between the direct and mapping forms of a factorized classical propagator. Journal of Chemical Physics, 2006, 124, 146103.	1.2	0
56	2SB1040 Theoretical Study on the Reaction Pathway and Free Energy of ATP Hydrolysis in Solution(2SB) Tj ETQq0 0 0 rgBT /Overlock 10 Butsuri, 2010, 50, S9.	0.0	0