Hisao Nakamura

List of Publications by Year
in descending order

54 papers	1,786 citations	236612 25 h-index	264894 42 g-index
54 all docs	54 docs citations	54 times ranked	1965 citing authors

#	Article	IF	Citations
1	Plasmon Resonance and Enhanced Near-Field of Anisotropic Nanoparticle Systems: Unified Analysis by Factorization of Light-Excited Dipole Distribution. Physical Chemistry Chemical Physics, 2022, 24, 2614-2622.	1.3	1
2	Thermoelectric and Thermal Properties of a (GeTe) 2 /Sb 2 Te 3 Interfacial Phaseâ€Change Memory Device. Physica Status Solidi - Rapid Research Letters, 2021, 15, 2000393.	1.2	1
3	Water Splitting Induced by Visible Light at a Copperâ€Based Singleâ€Molecule Junction. Small, 2021, 17, e2008109.	5.2	3
4	Probing embedded topological modes in bulk-like GeTe-Sb2Te3 heterostructures. Scientific Reports, 2020, 10, 21806.	1.6	2
5	Structural transition pathway and bipolar switching of the GeTeâ€“Sb₂Te₃ superlattice as interfacial phase-change memory. Faraday Discussions, 2019, 213, 303-319.	1.6	11
6	Phase-change memories (PCM) â€“ Experiments and modelling: general discussion. Faraday Discussions, 2019, 213, 393-420.	1.6	7
7	Identifying the molecular adsorption site of a single molecule junction through combined Raman and conductance studies. Chemical Science, 2019, 10, 6261-6269.	3.7	32
8	A Magnetoresistance Induced by a Nonzero Berry Phase in GeTe/Sb 2 Te 3 Chalcogenide Superlattices. Advanced Functional Materials, 2017, 27, 1702243.	7.8	24
9	Resistive switching mechanism of GeTeâ€“Sb₂Te₃ interfacial phase change memory and topological properties of embedded two-dimensional states. Nanoscale, 2017, 9, 9386-9395.	2.8	36
10	Resolving metal-molecule interfaces at single-molecule junctions. Scientific Reports, 2016, 6, 26606.	1.6	55
11	Theoretical Aspects of Quantum Transport and Computational Modeling of Molecular Electronic Device. , 2016, , 191-216.		0
12	The effect of a Ta oxygen scavenger layer on HfO₂-based resistive switching behavior: thermodynamic stability, electronic structure, and low-bias transport. Physical Chemistry Chemical Physics, 2016, 18, 7502-7510.	1.3	31
13	Competitive effects of oxygen vacancy formation and interfacial oxidation on an ultra-thin HfO₂-based resistive switching memory: beyond filament and charge hopping models. Physical Chemistry Chemical Physics, 2016, 18, 8820-8826.	1.3	22
14	Site-Selection in Single-Molecule Junction for Highly Reproducible Molecular Electronics. Journal of the American Chemical Society, 2016, 138, 1294-1300.	6.6	88
15	Adsorption Site Recognition in Single Molecular Junctions Spectroscopy. Hyomen Kagaku, 2016, 37, 288-293.	0.0	0
16	Temperature dependence of the thermopower and its variation of the Au atomic contact. Nanotechnology, 2015, 26, 045709.	1.3	4
17	A supercell approach to the doping effect on the thermoelectric properties of SnSe. Physical Chemistry Chemical Physics, 2015, 17, 29647-29654.	1.3	26
18	First-Principles Transport Modeling for Metal/Insulator/Metal Structures. , 2014, , .		1

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19	Design of ReRAM cell structure by metal buffer and contact engineering via first-principles transport calculations. , 2014, , .		1
20	Influence of surface polarity on water dynamics at the water/rutile TiO₂(110) interface. Journal of Physics Condensed Matter, 2014, 26, 244102.	0.7	30
21	(Invited) Non-Equilibrium Transport Theory Applied to Nano Electronics Problems. ECS Transactions, 2014, 64, 63-69.	0.3	1
22	Additive Electron Pathway and Nonadditive Molecular Conductance by Using a Multipodal Bridging Compound. Journal of Physical Chemistry C, 2014, 118, 5275-5283.	1.5	17
23	Single Molecular Resistive Switch Obtained via Sliding Multiple Anchoring Points and Varying Effective Wire Length. Journal of the American Chemical Society, 2014, 136, 7327-7332.	6.6	101
24	Universal Medium-Range Order of Amorphous Metal Oxides. Physical Review Letters, 2013, 111, 155502.	2.9	27
25	Controlling Formation of Single-Molecule Junctions by Electrochemical Reduction of Diazonium Terminal Groups. Journal of the American Chemical Society, 2013, 135, 3319-3322.	6.6	71
26	Polarizable Site Charge Model at Liquid/Solid Interfaces for Describing Surface Polarity: Application to Structure and Molecular Dynamics of Water/Rutile TiO₂(110) Interface. Journal of Chemical Theory and Computation, 2013, 9, 1193-1201.	2.3	29
27	Conductance and SERS Measurement of Benzenedithiol Molecules Bridging Between Au Electrodes. Journal of Physical Chemistry C, 2013, 117, 1791-1795.	1.5	47
28	Thermoelectric Efficiency of Organometallic Complex Wires via Quantum Resonance Effect and Long-Range Electric Transport Property. Journal of the American Chemical Society, 2013, 135, 16545-16552.	6.6	27
29	Ab initiotheory for current-induced molecular switching: Melamine on Cu(001). Physical Review B, 2013, 87, .	1.1	25
30	Long-Range Electron Transport of Ruthenium-Centered Multilayer Films via a Stepping-Stone Mechanism. ACS Nano, 2012, 6, 1988-1999.	7.3	62
31	First-principles study of electronic structure and charge transport at PTCDA molecular layers on Ag(111) and Al(111) electrodes. Physical Review B, 2011, 84, .	1.1	7
32	Nature of Electron Transport by Pyridine-Based Tripodal Anchors: Potential for Robust and Conductive Single-Molecule Junctions with Gold Electrodes. Journal of the American Chemical Society, 2011, 133, 3014-3022.	6.6	94
33	Inelastic Transport and Low-Bias Rectification in a Single-Molecule Diode. ACS Nano, 2011, 5, 8331-8339.	7.3	78
34	Switch of Conducting Orbital by Bias-Induced Electronic Contact Asymmetry in a Bipyrimidinyl-biphenyl Diblock Molecule: Mechanism to Achieve a pn Directional Molecular Diode. Journal of Physical Chemistry C, 2011, 115, 19931-19938.	1.5	48
35	Electron correlation enhancement of the diode property of asymmetric molecules. Physical Review B, 2011, 84, .	1.1	7
36	Theory and First Principles Calculation of Single Molecular Conductance with Electron-phonon Scattering. Hyomen Kagaku, 2011, 32, 622-628.	0.0	0

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37	DFT-Based Theoretical Calculations of Nb- and W-Doped Anatase TiO₂: Complex Formation between W Dopants and Oxygen Vacancies. Journal of Physical Chemistry C, 2010, 114, 12777-12783.	1.5	32
38	Effect of Anchoring Group Position on Formation and Conductance of a Single Disubstituted Benzene Molecule Bridging Au Electrodes: Change of Conductive Molecular Orbital and Electron Pathway. Journal of Physical Chemistry C, 2010, 114, 22254-22261.	1.5	86
39	First-Principles Study for Detection of Inelastic Electron Transport in Molecular Junctions by Internal Substitution. Journal of Physical Chemistry C, 2010, 114, 12280-12289.	1.5	20
40	First-principles study of charge-density waves on Cu surfaces covered by In, Pb, and Bi atoms: Analysis of electronic structure and surface phonons. Physical Review B, 2010, 82, .	1.1	1
41	First-Principle Calculations of Solvated Electrons at Protic Solventâ^'TiO₂ Interfaces with Oxygen Vacancies. Journal of Physical Chemistry C, 2009, 113, 7236-7245.	1.5	19
42	Systematic Study on Quantum Confinement and Waveguide Effects for Elastic and Inelastic Currents in Atomic Gold Wire:â€‰ Importance of the Phase Factor for Modeling Electrodes. Nano Letters, 2008, 8, 6-12.	4.5	23
43	Efficientab initiomethod for inelastic transport in nanoscale devices: Analysis of inelastic electron tunneling spectroscopy. Physical Review B, 2008, 78, .	1.1	39
44	Ab initiocalculations of inelastic transport in atomic/molecular junctions and waveguide effects. Journal of Physics Condensed Matter, 2008, 20, 224023.	0.7	4
45	Theoretical study of the photodesorption mechanism of nitric oxide on a Ag(111) surface: A nonequilibrium Greenâ€™s function approach to hot-electron tunneling. Journal of Chemical Physics, 2006, 125, 084708.	1.2	11
46	An efficient molecular orbital approach for self-consistent calculations of molecular junctions. Journal of Chemical Physics, 2006, 125, 194106.	1.2	23
47	Electron tunneling of photochemical reactions on metal surfaces: Nonequilibrium Greenâ€™s functionâ€“density functional theory approach to photon energy dependence of reaction probability. Journal of Chemical Physics, 2005, 122, 194706.	1.2	11
48	Extension of the fourfold way for calculation of global diabatic potential energy surfaces of complex, multiarrangement, non-Bornâ€“Oppenheimer systems:â€‚Application to HNCO(S0,S1). Journal of Chemical Physics, 2003, 118, 6816-6829.	1.2	108
49	Direct diabatization of electronic states by the fourfold way. II. Dynamical correlation and rearrangement processes. Journal of Chemical Physics, 2002, 117, 5576-5593.	1.2	156
50	The direct calculation of diabatic states based on configurational uniformity. Journal of Chemical Physics, 2001, 115, 10353.	1.2	187
51	K-1926 Effect of Injection Rate and Fuel Property on the Combustion Characteristics in a Direct-Injection Gasoline Engine. The Proceedings of the JSME Annual Meeting, 2001, II.01.1, 485-486.	0.0	0
52	State resolved reaction rates of the spin-forbidden predissociation of N2O: A quantum dynamics study of the rotational effect. Journal of Chemical Physics, 2000, 112, 1785-1796.	1.2	10
53	Theoretical study on the spin-forbidden predissociation reaction of N2O: Ab initio potential energy surfaces and quantum dynamics calculations. Journal of Chemical Physics, 1999, 110, 9937-9947.	1.2	30
54	Quantum calculation of the vibrational energy level structure of N2O based on ab initio potential surface. Chemical Physics Letters, 1998, 297, 187-192.	1.2	10