Stefano Corni

List of Publications by Year
in descending order

194	7,436	53939 47	75989 78
papers	citations	h-index	g-index

199	199	199	7993
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Insight on Chirality Encoding from Small Thiolated Molecule to Plasmonic Au@Ag and Au@Au Nanoparticles. ACS Nano, 2022, 16, 1089-1101.	7.3	25
2	High affinity protein surface binding through co-engineering of nanoparticles and proteins. Nanoscale, 2022, 14, 2411-2418.	2.8	7
3	Atomistic Simulations of Functionalized Nano-Materials for Biosensors Applications. International Journal of Molecular Sciences, 2022, 23, 1484.	1.8	7
4	Role of Ionic Strength in the Formation of Stable Supramolecular Nanoparticleâ€“Protein Conjugates for Biosensing. International Journal of Molecular Sciences, 2022, 23, 2368.	1.8	5
5	Exploring AuRh Nanoalloys: A Computational Perspective on the Formation and Physical Properties. ChemPhysChem, 2022, 23, .	1.0	6
6	Engineering the Aggregation of Dyes on Ligand-Shell Protected Gold Nanoparticles to Promote Plexcitons Formation. Nanomaterials, 2022, 12, 1180.	1.9	7
7	Electronic Dynamics of a Molecular System Coupled to a Plasmonic Nanoparticle Combining the Polarizable Continuum Model and Many-Body Perturbation Theory. Journal of Physical Chemistry C, 2022, 126, 8768-8776.	1.5	3
8	Inverted Conformation Stability of a Motor Molecule on a Metal Surface. Journal of Physical Chemistry C, 2022, 126, 9034-9040.	1.5	5
9	Acidic pH Promotes Refolding and Macroscopic Assembly of Amyloid Î² (16â€“22) Peptides at the Airâ€“Water Interface. Journal of Physical Chemistry Letters, 2022, 13, 6674-6679.	2.1	3
10	Proline isomerization effects in the amyloidogenic protein Î²₂-microglobulin. Physical Chemistry Chemical Physics, 2021, 23, 356-367.	1.3	8
11	Selective switching of multiple plexcitons in colloidal materials: directing the energy flow at the nanoscale. Nanoscale, 2021, 13, 6005-6015.	2.8	12
12	Quantum optimal control with quantum computers: A hybrid algorithm featuring machine learning optimization. Physical Review A, 2021, 103, .	1.0	13
13	Molecular Dynamics Simulations of a Catalytic Multivalent Peptideâ€“Nanoparticle Complex. International Journal of Molecular Sciences, 2021, 22, 3624.	1.8	13
14	Exploring the Spatial Features of Electronic Transitions in Molecular and Biomolecular Systems by Swift Electrons. Journal of Chemical Theory and Computation, 2021, 17, 2364-2373.	2.3	1
15	Study of the Rate-Determining Step of Rh Catalyzed CO2 Reduction: Insight on the Hydrogen Assisted Molecular Dissociation. Catalysts, 2021, 11, 538.	1.6	6
16	Lanthanide Ions Sensitization by Small Noble Metal Nanoclusters. ACS Photonics, 2021, 8, 1364-1376.	3.2	6
17	LayerPCM: An implicit scheme for dielectric screening from layered substrates. Journal of Chemical Physics, 2021, 154, 224114.	1.2	11
18	Strong Coupling between Localized Surface Plasmons and Molecules by Coupled Cluster Theory. Nano Letters, 2021, 21, 6664-6670.	4.5	32

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19	Time-Resolved Excited-State Analysis of Molecular Electron Dynamics by TDDFT and Betheâ€“Salpeter Equation Formalisms. Journal of Chemical Theory and Computation, 2021, 17, 6314-6329.	2.3	8
20	Atomistic simulations of gold surface functionalization for nanoscale biosensors applications. Nanotechnology, 2021, 32, 095702.	1.3	9
21	Quantum computing for classical problems: variational quantum eigensolver for activated processes. New Journal of Physics, 2021, 23, 123045.	1.2	5
22	Role of metal-nanostructure features on tip-enhanced photoluminescence of single molecules. Journal of Chemical Physics, 2021, 155, 214304.	1.2	6
23	Strong Coupling with Light Enhances the Photoisomerization Quantum Yield of Azobenzene. CheM, 2020, 6, 250-265.	5.8	59
24	Investigating ultrafast two-pulse experiments on single DNQDI fluorophores: a stochastic quantum approach. Physical Chemistry Chemical Physics, 2020, 22, 16734-16746.	1.3	8
25	Real-time dynamics of plasmonic resonances in nanoparticles described by a boundary element method with generic dielectric function. Journal of Chemical Physics, 2020, 153, 184114.	1.2	13
26	Hybrid theoretical models for molecular nanoplasmonics. Journal of Chemical Physics, 2020, 153, 200901.	1.2	27
27	Effects of Ligand Binding on the Energy Landscape of Acyl-CoA-Binding Protein. Biophysical Journal, 2020, 119, 1821-1832.	0.2	15
28	Adsorption and Motion of Single Molecular Motors on TiO2(110). Journal of Physical Chemistry C, 2020, 124, 24776-24785.	1.5	5
29	An open quantum system theory for polarizable continuum models. Journal of Chemical Physics, 2020, 152, 174114.	1.2	14
30	Simulating Plasmon Resonances of Gold Nanoparticles with Bipyramidal Shapes by Boundary Element Methods. Journal of Chemical Theory and Computation, 2020, 16, 3807-3815.	2.3	15
31	Plasmonic Resonances of Metal Nanoparticles: Atomistic vs. Continuum Approaches. Frontiers in Chemistry, 2020, 8, 340.	1.8	23
32	Atomistic insight into the aggregation of [Au₂₅(SR)₁₈]^q nanoclusters. Nanoscale Advances, 2020, 2, 2842-2852.	2.2	6
33	Octopus, a computational framework for exploring light-driven phenomena and quantum dynamics in extended and finite systems. Journal of Chemical Physics, 2020, 152, 124119.	1.2	210
34	Photochemistry in the strong coupling regime: A trajectory surface hopping scheme. Journal of Computational Chemistry, 2020, 41, 2033-2044.	1.5	25
35	Low-Resolution Models for the Interaction Dynamics of Coated Gold Nanoparticles with Î²2-microglobulin. International Journal of Molecular Sciences, 2019, 20, 3866.	1.8	10
36	Role of coherence in the plasmonic control of molecular absorption. Journal of Chemical Physics, 2019, 151, 044703.	1.2	14

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37	Water splitting of hydrogen chemisorbed in graphene oxide dynamically evolves into a graphane lattice. Carbon, 2019, 153, 234-241.	5.4	12
38	III-V semicondutor nanostructures and iontronics: InAs nanowire-based electric double layer field effect transistors. AIP Conference Proceedings, 2019, , .	0.3	4
39	Quantifying the Plasmonic Character of Optical Excitations in a Molecular J-Aggregate. Journal of Chemical Theory and Computation, 2019, 15, 3197-3203.	2.3	9
40	Nonequilibrium Solvent Polarization Effects in Real-Time Electronic Dynamics of Solute Molecules Subject to Time-Dependent Electric Fields: A New Feature of the Polarizable Continuum Model. Journal of Chemical Theory and Computation, 2019, 15, 2306-2319.	2.3	9
41	Interplay between Intra- and Intermolecular Charge Transfer in the Optical Excitations of J-Aggregates. Journal of Physical Chemistry C, 2019, 123, 6831-6838.	1.5	20
42	Evidence of a Thermodynamic Ramp for Hole Hopping to Protect a Redox Enzyme from Oxidative Damage. Journal of Physical Chemistry Letters, 2019, 10, 1450-1456.	2.1	10
43	Multiscale modelling of photoinduced processes in composite systems. Nature Reviews Chemistry, 2019, 3, 315-330.	13.8	78
44	Tip-Enhanced Infrared Difference-Nanospectroscopy of the Proton Pump Activity of Bacteriorhodopsin in Single Purple Membrane Patches. Nano Letters, 2019, 19, 3104-3114.	4.5	36
45	A classical picture of subnanometer junctions: an atomistic Drude approach to nanoplasmonics. Nanoscale, 2019, 11, 6004-6015.	2.8	25
46	Quantum optimal control theory for solvated systems. Journal of Chemical Physics, 2019, 151, 194109.	1.2	8
47	Difference mid-IR nanospectroscopy on individual patches of purple membranes: the proton pump activity of bacteriorhodopsin at the nanoscale. , 2019, , .		0
48	The interaction of peptides and proteins with nanostructures surfaces: a challenge for nanoscience. Current Opinion in Colloid and Interface Science, 2019, 41, 86-94.	3.4	35
49	Citrate stabilized gold nanoparticles interfere with amyloid fibril formation: D76N and Î”N6 Î²2-microglobulin variants. Nanoscale, 2018, 10, 4793-4806.	2.8	30
50	Density-Dependent Formulation of Dispersionâ€“Repulsion Interactions in Hybrid Multiscale Quantum/Molecular Mechanics (QM/MM) Models. Journal of Chemical Theory and Computation, 2018, 14, 1671-1681.	2.3	24
51	Adsorption Mechanisms of Nucleobases on the Hydrated Au(111) Surface. Langmuir, 2018, 34, 14749-14756.	1.6	9
52	Enhanced light-harvesting of protein-pigment complexes assisted by a quantum dot antenna. , 2018, , .		0
53	Manipulating azobenzene photoisomerization through strong lightâ€“molecule coupling. Nature Communications, 2018, 9, 4688.	5.8	111
54	Angle-resolved photoemission spectroscopy from first-principles quantum Monte Carlo. Journal of Chemical Physics, 2018, 149, 154102.	1.2	1

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55	Solid-State Effects on the Optical Excitation of Pushâ€“Pull Molecular J-Aggregates by First-Principles Simulations. ACS Omega, 2018, 3, 10481-10486.	1.6	15
56	Probing quantum coherence in ultrafast molecular processes: An ab initio approach to open quantum systems. Journal of Chemical Physics, 2018, 148, 204112.	1.2	18
57	Role of Organic Ligands Orientation on the Geometrical and Optical Properties of Au₂₅(SCH₃)₁₈⁰. Journal of Physical Chemistry A, 2018, 122, 6864-6872.	1.1	9
58	Shaping excitons in light-harvesting proteins through nanoplasmonics. Chemical Science, 2018, 9, 6219-6227.	3.7	9
59	Citrate-stabilized gold nanoparticles hinder fibrillogenesis of a pathological variant of Î²₂-microglobulin. Nanoscale, 2017, 9, 3941-3951.	2.8	26
60	Equation of motion for the solvent polarization apparent charges in the polarizable continuum model: Application to time-dependent CI. Journal of Chemical Physics, 2017, 146, 064116.	1.2	14
61	Fibrillation-prone conformations of the amyloid-Î²-42 peptide at the gold/water interface. Nanoscale, 2017, 9, 2279-2290.	2.8	25
62	Reply to â€œMolecular mechanics models for the image chargeâ€. Journal of Computational Chemistry, 2017, 38, 2130-2133.	1.5	2
63	Carbon nanotubes as excitonic insulators. Nature Communications, 2017, 8, 1461.	5.8	51
64	How To Identify Plasmons from the Optical Response of Nanostructures. ACS Nano, 2017, 11, 7321-7335.	7.3	72
65	Excitation energy-transfer in functionalized nanoparticles: Going beyond the FÃ¶rster approach. Journal of Chemical Physics, 2016, 144, 074101.	1.2	6
66	Modeling and simulation of proteinâ€“surface interactions: achievements and challenges. Quarterly Reviews of Biophysics, 2016, 49, e4.	2.4	163
67	First-Principle Molecular Dynamics of Sliding Diamond Surfaces: Tribochemical Reactions with Water and Load Effects. Journal of Low Temperature Physics, 2016, 185, 174-182.	0.6	9
68	A dynamical coarse-grained model to disclose allosteric control of misfolding Î²2-microglobulin. RSC Advances, 2016, 6, 93111-93118.	1.7	3
69	Correlation Effects in Scanning Tunneling Microscopy Images of Molecules Revealed by Quantum Monte Carlo. Journal of Chemical Theory and Computation, 2016, 12, 5339-5349.	2.3	5
70	Real-Time Description of the Electronic Dynamics for a Molecule Close to a Plasmonic Nanoparticle. Journal of Physical Chemistry C, 2016, 120, 28774-28781.	1.5	34
71	Predicting signatures of anisotropic resonance energy transfer in dye-functionalized nanoparticles. RSC Advances, 2016, 6, 104648-104656.	1.7	1
72	Extending the essential dynamics analysis to investigate molecular properties: application to the redox potential of proteins. Physical Chemistry Chemical Physics, 2016, 18, 18450-18459.	1.3	18

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73	The interaction with gold suppresses fiber-like conformations of the amyloid Î² (16â€“22) peptide. Nanoscale, 2016, 8, 8737-8748.	2.8	55
74	A dynamical approach to non-adiabatic electron transfers at the bio-inorganic interface. Physical Chemistry Chemical Physics, 2016, 18, 10538-10549.	1.3	11
75	Quantifying the Plasmonic Character of Optical Excitations in Nanostructures. ACS Photonics, 2016, 3, 520-525.	3.2	51
76	Modeling solvation effects in real-space and real-time within density functional approaches. Journal of Chemical Physics, 2015, 143, 144111.	1.2	10
77	Influence of size, shape and coreâ€“shell interface on surface plasmon resonance in Ag and Ag@MgO nanoparticle films deposited on Si/SiO x. Beilstein Journal of Nanotechnology, 2015, 6, 404-413.	1.5	17
78	Distance-Based Configurational Entropy of Proteins from Molecular Dynamics Simulations. PLoS ONE, 2015, 10, e0132356.	1.1	32
79	Equation of Motion for the Solvent Polarization Apparent Charges in the Polarizable Continuum Model: Application to Real-Time TDDFT. Journal of Physical Chemistry A, 2015, 119, 5405-5416.	1.1	43
80	Probing the Influence of Citrate-Capped Gold Nanoparticles on an Amyloidogenic Protein. ACS Nano, 2015, 9, 2600-2613.	7.3	80
81	Non-linear optical response by functionalized gold nanospheres: identifying design principles to maximize the molecular photo-release. Nanoscale, 2015, 7, 13345-13357.	2.8	10
82	Facet selectivity in gold binding peptides: exploiting interfacial water structure. Chemical Science, 2015, 6, 5204-5214.	3.7	68
83	Can Azobenzene Photoisomerize When Chemisorbed on a Gold Surface? An Analysis of Steric Effects Based on Nonadiabatic Dynamics Simulations. Journal of Physical Chemistry C, 2015, 119, 5962-5974.	1.5	21
84	Affinity and Selectivity of Peptides for Inorganic Materials: A Thermodynamic Discussion of the Role of Conformational Flexibility. Jom, 2015, 67, 781-787.	0.9	2
85	A few key residues determine the high redox potential shift in azurin mutants. Organic and Biomolecular Chemistry, 2015, 13, 11003-11013.	1.5	35
86	High stability and sensitivity of gold nano-islands for localized surface plasmon spectroscopy: Role of solvent viscosity and morphology. Sensors and Actuators B: Chemical, 2014, 191, 356-363.	4.0	9
87	Work Function Changes of Azo-Derivatives Adsorbed on a Gold Surface. Journal of Physical Chemistry C, 2014, 118, 26033-26040.	1.5	9
88	Quenching of the Photoisomerization of Azobenzene Self-Assembled Monolayers by the Metal Substrate. Journal of Physical Chemistry C, 2014, 118, 25906-25917.	1.5	14
89	Interaction with a Gold Surface Reshapes the Free Energy Landscape of Alanine Dipeptide. Journal of Physical Chemistry C, 2014, 118, 11357-11364.	1.5	29
90	van der Waals effects at molecule-metal interfaces. Physical Review B, 2014, 90, .	1.1	22

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91	Surface Packing Determines the Redox Potential Shift of Cytochrome c Adsorbed on Gold. Journal of the American Chemical Society, 2014, 136, 12929-12937.	6.6	39
92	Charge Transfer Rates at a Bioâ€“Inorganic Interface. Journal of Physical Chemistry C, 2014, 118, 18820-18828.	1.5	3
93	Enthalpyâ€“Entropy Tuning in the Adsorption of Nucleobases at the Au(111) Surface. Journal of Chemical Theory and Computation, 2014, 10, 1707-1716.	2.3	36
94	Can small hydrophobic gold nanoparticles inhibit Î²₂-microglobulin fibrillation?. Nanoscale, 2014, 6, 7903-7911.	2.8	37
95	Light-Induced Field Enhancement in Nanoscale Systems from First-Principles: The Case of Polyacenes. ACS Photonics, 2014, 1, 1049-1058.	3.2	47
96	The cavity electromagnetic field within the polarizable continuum model of solvation: An application to the real-time time dependent density functional theory. Computational and Theoretical Chemistry, 2014, 1040-1041, 112-119.	1.1	19
97	The cavity electromagnetic field within the polarizable continuum model of solvation. Journal of Chemical Physics, 2014, 140, 164114.	1.2	23
98	Wettability of Azobenzene Self-Assembled Monolayers. Langmuir, 2014, 30, 4415-4421.	1.6	5
99	Conformational Behavior of Genetically-Engineered Dodecapeptides as a Determinant of Binding Affinity for Gold.. Journal of Physical Chemistry C, 2013, 117, 16990-17003.	1.5	52
100	GolP-CHARMM: First-Principles Based Force Fields for the Interaction of Proteins with Au(111) and Au(100). Journal of Chemical Theory and Computation, 2013, 9, 1616-1630.	2.3	210
101	Reactivity of the ZnS(101Ì…0) Surface to Small Organic Ligands by Density Functional Theory. Journal of Physical Chemistry C, 2013, 117, 16034-16041.	1.5	6
102	Interaction of Nucleic Acid Bases with the Au(111) Surface. Journal of Chemical Theory and Computation, 2013, 9, 4552-4561.	2.3	33
103	Structural Properties of Azobenzene Self-Assembled Monolayers by Atomistic Simulations. Langmuir, 2013, 29, 10505-10512.	1.6	13
104	Plasmon-Controlled Light-Harvesting: Design Rules for Biohybrid Devices via Multiscale Modeling. Nano Letters, 2013, 13, 4475-4484.	4.5	35
105	How the Dynamics of the Metal-Binding Loop Region Controls the Acid Transition in Cupredoxins. Biochemistry, 2013, 52, 7397-7404.	1.2	5
106	Dynamical Treatment of Charge Transfer through Duplex Nucleic Acids Containing Modified Adenines. ACS Nano, 2013, 7, 9396-9406.	7.3	8
107	Exciton Transfer of Azobenzene Derivatives in Self-Assembled Monolayers. Journal of Physical Chemistry C, 2013, 117, 25026-25041.	1.5	16
108	First-Principles-Based Force Field for the Interaction of Proteins with Au(100)(5â€‰Ã—â€‰1): An Extension of GolP-CHARMM. Journal of Physical Chemistry C, 2013, 117, 24292-24306.	1.5	61

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109	Single-Molecule Folding Mechanism of an EF-Hand Neuronal Calcium Sensor. Structure, 2013, 21, 1812-1821.	1.6	27
110	Can we control the electronic energy transfer in molecular dyads through metal nanoparticles? A QM/continuum investigation. Physical Chemistry Chemical Physics, 2013, 15, 3294.	1.3	18
111	Simulation of Proteinâ€“Surface Interactions by a Coarse-Grained Method. BioNanoScience, 2013, 3, 12-20.	1.5	5
112	Cytochrome C on a gold surface: investigating structural relaxations and their role in proteinâ€“surface electron transfer by molecular dynamics simulations. Physical Chemistry Chemical Physics, 2013, 15, 5945.	1.3	20
113	Benchmarking Common Approximations for Determining the Particle-Size Dependence of Adsorbate-Induced Localized Surface Plasmon Resonance Shifts. Journal of Physical Chemistry C, 2013, 117, 14742-14750.	1.5	6
114	Self-Assembly of Mono- And Bidentate Oligoarylene Thiols onto Polycrystalline Au. Langmuir, 2013, 29, 13198-13208.	1.6	19
115	Modeling opto-electronic properties of a dye molecule in proximity of a semiconductor nanoparticle. Journal of Chemical Physics, 2013, 139, 024105.	1.2	16
116	The Active Site Loop Modulates the Reorganization Energy of Blue Copper Proteins by Controlling the Dynamic Interplay with Solvent. Journal of Physical Chemistry Letters, 2013, 4, 710-715.	2.1	25
117	Load-Induced Confinement Activates Diamond Lubrication by Water. Physical Review Letters, 2013, 111, 146101.	2.9	91
118	Proposed Alteration of Images of Molecular Orbitals Obtained Using a Scanning Tunneling Microscope as a Probe of Electron Correlation. Physical Review Letters, 2013, 110, 018305.	2.9	9
119	The Structure of Neuronal Calcium Sensor-1 in Solution Revealed by Molecular Dynamics Simulations. PLoS ONE, 2013, 8, e74383.	1.1	12
120	First principle evaluation of the chiroptical activity of the di-phenyl-diazene derivatives. Journal of Chemical Physics, 2012, 137, 124307.	1.2	4
121	Optical Excitations and Field Enhancement in Short Graphene Nanoribbons. Journal of Physical Chemistry Letters, 2012, 3, 924-929.	2.1	32
122	First-principle-based MD description of azobenzene molecular rods. Theoretical Chemistry Accounts, 2012, 131, 1.	0.5	18
123	A Density Functional Theory Study of Cytosine on Au(111). Journal of Physical Chemistry C, 2012, 116, 21366-21373.	1.5	38
124	Docking of Ubiquitin to Gold Nanoparticles. ACS Nano, 2012, 6, 9863-9878.	7.3	131
125	Proteins and Peptides at Gold Surfaces: Insights from Atomistic Simulations. ACS Symposium Series, 2012, , 229-250.	0.5	8
126	Formation energy of dangling bonds on hydrogenated diamond surfaces: A first-principles study. Physical Review B, 2012, 85, .	1.1	5

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127	The Reversible Opening of Water Channels in Cytochrome c Modulates the Heme Iron Reduction Potential. Journal of the American Chemical Society, 2012, 134, 13670-13678.	6.6	71
128	Low-lying electronic excitations and optical absorption spectra of the black dye sensitizer: a first-principles study. Theoretical Chemistry Accounts, 2012, 131, 1.	0.5	9
129	Anomalous Wetting Layer at the Au(111) Surface. Journal of Physical Chemistry Letters, 2011, 2, 2582-2586.	2.1	50
130	The Reorganization Energy in Cytochrome c is Controlled by the Accessibility of the Heme to the Solvent. Journal of Physical Chemistry Letters, 2011, 2, 1761-1765.	2.1	57
131	Surface-Enhanced Fluorescence within a Metal Nanoparticle Array: The Role of Solvent and Plasmon Couplings. Journal of Physical Chemistry C, 2011, 115, 5450-5460.	1.5	46
132	Simulation of Peptideâ€“Surface Recognition. Journal of Physical Chemistry Letters, 2011, 2, 1510-1519.	2.1	67
133	Peptide Synthesis of Gold Nanoparticles: The Early Steps of Gold Reduction Investigated by Density Functional Theory. Nano Letters, 2011, 11, 1313-1318.	4.5	32
134	Direct monitoring of opto-mechanical switching of self-assembled monolayer films containing the azobenzene group. Beilstein Journal of Nanotechnology, 2011, 2, 834-844.	1.5	18
135	Interaction of Î²-Sheet Folds with a Gold Surface. PLoS ONE, 2011, 6, e20925.	1.1	61
136	Visualizing electron correlation by means of ab initio scanning tunneling spectroscopy images of single molecules. Journal of Chemical Physics, 2011, 134, 024104.	1.2	12
137	Proteinâ€“surface interactions: challenging experiments and computations. Journal of Molecular Recognition, 2010, 23, 259-262.	1.1	41
138	The Conformations of Amino Acids on a Gold(111) Surface. ChemPhysChem, 2010, 11, 1763-1767.	1.0	59
139	ProMetCS: An Atomistic Force Field for Modeling Proteinâ^'Metal Surface Interactions in a Continuum Aqueous Solvent. Journal of Chemical Theory and Computation, 2010, 6, 1753-1768.	2.3	58
140	Hydroxyl-Rich Î²-Sheet Adhesion to the Gold Surface in Water by First-Principle Simulations. Journal of the American Chemical Society, 2010, 132, 4790-4795.	6.6	55
141	Quantum Mechanical Approach to Solvent Effects on the Optical Properties of Metal Nanoparticles and Their Efficiency As Excitation Energy Transfer Acceptors. Journal of Physical Chemistry C, 2010, 114, 1553-1561.	1.5	16
142	Water Adsorption on Native and Hydrogenated Diamond (001) Surfaces. Journal of Physical Chemistry C, 2010, 114, 7045-7053.	1.5	47
143	Interaction of Amino Acids with the Au(111) Surface: Adsorption Free Energies from Molecular Dynamics Simulations. Langmuir, 2010, 26, 8347-8351.	1.6	185
144	GolP: An atomistic forceâ€field to describe the interaction of proteins with Au(111) surfaces in water. Journal of Computational Chemistry, 2009, 30, 1465-1476.	1.5	237

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145	Nonplasmonic Metal Particles as Excitation Energy Transfer Acceptors: an Unexpected Efficiency Revealed by Quantum Mechanics. Journal of Physical Chemistry C, 2009, 113, 16364-16370.	1.5	21
146	First Principles Effective Electronic Couplings for Hole Transfer in Natural and Size-Expanded DNA. Journal of Physical Chemistry B, 2009, 113, 9402-9415.	1.2	64
147	Fluorescence Enhancement of Chromophores Close to Metal Nanoparticles. Optimal Setup Revealed by the Polarizable Continuum Model. Journal of Physical Chemistry C, 2009, 113, 121-133.	1.5	141
148	Including image charge effects in the molecular dynamics simulations of molecules on metal surfaces. Journal of Computational Chemistry, 2008, 29, 1656-1666.	1.5	109
149	Unraveling the Interaction between Histidine Side Chain and the Au(111) Surface: A DFT Study. Journal of Physical Chemistry C, 2008, 112, 13540-13545.	1.5	62
150	A Theoretical Study of the Electrochemical Gate Effect in an STM-Based Biomolecular Transistor. IEEE Nanotechnology Magazine, 2007, 6, 561-570.	1.1	16
151	Water-Mediated Electron Transfer between Protein Redox Centers. Journal of Physical Chemistry B, 2007, 111, 3774-3781.	1.2	27
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153	Studying SERS from Metal Nanoparticles and Nanoparticles Aggregates with Continuum Models. , 2006, , 105-123.		5
154	Formation and relaxation of excited states in solution: A new time dependent polarizable continuum model based on time dependent density functional theory. Journal of Chemical Physics, 2006, 124, 124520.	1.2	484
155	First-principles density-functional theory calculations of electron-transfer rates in azurin dimers. Journal of Chemical Physics, 2006, 124, 064501.	1.2	42
156	A combined Raman, DFT and MD study of the solvation dynamics and the adsorption process of pyridine in silver hydrosols. Physical Chemistry Chemical Physics, 2006, 8, 171-178.	1.3	38
157	Unravelling single metalloprotein electron transfer by scanning probe techniques. Physical Chemistry Chemical Physics, 2006, 8, 4383.	1.3	105
158	Semiempirical (ZINDO-PCM) Approach to Predict the Radiative and Nonradiative Decay Rates of a Molecule Close to Metal Particles. Journal of Physical Chemistry B, 2006, 110, 16652-16659.	1.2	25
159	Water Effects on Electron Transfer in Azurin Dimers. Journal of Physical Chemistry B, 2006, 110, 23796-23800.	1.2	16
160	A new algorithm for rigid body molecular dynamics. Chemical Physics, 2006, 328, 259-268.	0.9	14
161	Self-consistent quantum mechanical model for the description of excitation energy transfers in molecules at interfaces. Journal of Chemical Physics, 2006, 125, 054710.	1.2	14
162	Studying SERS from Metal Nanoparticlesand Nanoparticles Aggregateswith Continuum Models. , 2006, , 105-124.		0

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163	Towards Protein Field-Effect Transistors: Report and Model of a Prototype. Advanced Materials, 2005, 17, 816-822.	11.1	84
164	Computational approach to study electron-transfer proteins: Azurin for bio-molecular devices. Computer Physics Communications, 2005, 169, 9-13.	3.0	5
165	Role of the electronic properties of azurin active site in the electron-transfer process. International Journal of Quantum Chemistry, 2005, 102, 328-342.	1.0	24
166	Infrared linear dichroism in stretched films: Quantum mechanical approach within the polarizable continuum model. International Journal of Quantum Chemistry, 2005, 104, 716-726.	1.0	9
167	Azurin for Biomolecular Electronics: a Reliability Study. Japanese Journal of Applied Physics, 2005, 44, 6864-6866.	0.8	6
168	Retention of nativelike conformation by proteins embedded in high external electric fields. Journal of Chemical Physics, 2005, 122, 181102.	1.2	13
169	Electronic excitation energies of molecules in solution within continuum solvation models: Investigating the discrepancy between state-specific and linear-response methods. Journal of Chemical Physics, 2005, 123, 134512.	1.2	187
170	Electronic excitation energies of molecules in solution: State specific and linear response methods for nonequilibrium continuum solvation models. Journal of Chemical Physics, 2005, 122, 104513.	1.2	271
171	The Reorganization Energy of Azurin in Bulk Solution and in the Electrochemical Scanning Tunneling Microscopy Setup. Journal of Physical Chemistry B, 2005, 109, 3423-3430.	1.2	38
172	A polarizable continuum model for molecules at diffuse interfaces. Journal of Chemical Physics, 2004, 120, 3893-3907.	1.2	66
173	Radiative and nonradiative decay rates of a molecule close to a metal particle of complex shape. Journal of Chemical Physics, 2004, 121, 10190-10202.	1.2	77
174	Second-order MÃ¸llerâ€“Plesset second derivatives for the polarizable continuum model: theoretical bases and application to solvent effects in electrophilic bromination of ethylene. Theoretical Chemistry Accounts, 2004, 111, 66-77.	0.5	13
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