Stefano Corni

List of Publications by Year
in descending order

194	7,436	47006	66911
papers	citations	47 h-index	78 g-index

199	199	199	6984
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	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.	3.0	484
2	Molecular properties in solution described with a continuum solvation model. Physical Chemistry Chemical Physics, 2002, 4, 5697-5712.	2.8	277
3	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.	3.0	271
4	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.	3.3	237
5	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.	5.3	210
6	Octopus, a computational framework for exploring light-driven phenomena and quantum dynamics in extended and finite systems. Journal of Chemical Physics, 2020, 152, 124119.	3.0	210
7	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.	3.0	187
8	Interaction of Amino Acids with the Au(111) Surface: Adsorption Free Energies from Molecular Dynamics Simulations. Langmuir, 2010, 26, 8347-8351.	3.5	185
9	Modeling and simulation of proteinâ€“surface interactions: achievements and challenges. Quarterly Reviews of Biophysics, 2016, 49, e4.	5.7	163
10	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.	3.1	141
11	Docking of Ubiquitin to Gold Nanoparticles. ACS Nano, 2012, 6, 9863-9878.	14.6	131
12	Enhanced response properties of a chromophore physisorbed on a metal particle. Journal of Chemical Physics, 2001, 114, 3739-3751.	3.0	122
13	Surface enhanced Raman scattering from a single molecule adsorbed on a metal particle aggregate: A theoretical study. Journal of Chemical Physics, 2002, 116, 1156-1164.	3.0	116
14	Manipulating azobenzene photoisomerization through strong lightâ€“molecule coupling. Nature Communications, 2018, 9, 4688.	12.8	111
15	Including image charge effects in the molecular dynamics simulations of molecules on metal surfaces. Journal of Computational Chemistry, 2008, 29, 1656-1666.	3.3	109
16	Unravelling single metalloprotein electron transfer by scanning probe techniques. Physical Chemistry Chemical Physics, 2006, 8, 4383.	2.8	105
17	Load-Induced Confinement Activates Diamond Lubrication by Water. Physical Review Letters, 2013, 111, 146101.	7.8	91
18	Towards Protein Field-Effect Transistors: Report and Model of a Prototype. Advanced Materials, 2005, 17, 816-822.	21.0	84

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19	Vibrational Circular Dichroism within the Polarizable Continuum Model:Â A Theoretical Evidence of Conformation Effects and Hydrogen Bonding for (S)-(âˆ')-3-Butyn-2-ol in CCl4Solution. Journal of Physical Chemistry A, 2002, 106, 12331-12339.	2.5	83
20	On the Calculation of Infrared Intensities in Solution within the Polarizable Continuum Model. Journal of Physical Chemistry A, 2000, 104, 9874-9879.	2.5	81
21	Probing the Influence of Citrate-Capped Gold Nanoparticles on an Amyloidogenic Protein. ACS Nano, 2015, 9, 2600-2613.	14.6	80
22	Multiscale modelling of photoinduced processes in composite systems. Nature Reviews Chemistry, 2019, 3, 315-330.	30.2	78
23	Radiative and nonradiative decay rates of a molecule close to a metal particle of complex shape. Journal of Chemical Physics, 2004, 121, 10190-10202.	3.0	77
24	How To Identify Plasmons from the Optical Response of Nanostructures. ACS Nano, 2017, 11, 7321-7335.	14.6	72
25	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.	13.7	71
26	Excitation energies of a molecule close to a metal surface. Journal of Chemical Physics, 2002, 117, 7266-7278.	3.0	70
27	Nonequilibrium formulation of infrared frequencies and intensities in solution: Analytical evaluation within the polarizable continuum model. Journal of Chemical Physics, 2000, 113, 11270-11279.	3.0	69
28	Facet selectivity in gold binding peptides: exploiting interfacial water structure. Chemical Science, 2015, 6, 5204-5214.	7.4	68
29	Simulation of Peptideâ€"Surface Recognition. Journal of Physical Chemistry Letters, 2011, 2, 1510-1519.	4.6	67
30	A polarizable continuum model for molecules at diffuse interfaces. Journal of Chemical Physics, 2004, 120, 3893-3907.	3.0	66
31	First Principles Effective Electronic Couplings for Hole Transfer in Natural and Size-Expanded DNA. Journal of Physical Chemistry B, 2009, 113, 9402-9415.	2.6	64
32	Unraveling the Interaction between Histidine Side Chain and the Au(111) Surface: A DFT Study. Journal of Physical Chemistry C, 2008, 112, 13540-13545.	3.1	62
33	Interaction of Î²-Sheet Folds with a Gold Surface. PLoS ONE, 2011, 6, e20925.	2.5	61
34	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.	3.1	61
35	The Conformations of Amino Acids on a Gold(111) Surface. ChemPhysChem, 2010, 11, 1763-1767.	2.1	59
36	Strong Coupling with Light Enhances the Photoisomerization Quantum Yield of Azobenzene. CheM, 2020, 6, 250-265.	11.7	59

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37	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.	5.3	58
38	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.	4.6	57
39	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.	13.7	55
40	The interaction with gold suppresses fiber-like conformations of the amyloid Î² (16â€"22) peptide. Nanoscale, 2016, 8, 8737-8748.	5.6	55
41	Theoretical Approach to the Calculation of Vibrational Raman Spectra in Solution within the Polarizable Continuum Model. Journal of Physical Chemistry A, 2001, 105, 8310-8316.	2.5	53
42	Conformational Behavior of Genetically-Engineered Dodecapeptides as a Determinant of Binding Affinity for Gold.. Journal of Physical Chemistry C, 2013, 117, 16990-17003.	3.1	52
43	Quantifying the Plasmonic Character of Optical Excitations in Nanostructures. ACS Photonics, 2016, 3, 520-525.	6.6	51
44	Carbon nanotubes as excitonic insulators. Nature Communications, 2017, 8, 1461.	12.8	51
45	Theoretical evaluation of Raman spectra and enhancement factors for a molecule adsorbed on a complex-shaped metal particle. Chemical Physics Letters, 2001, 342, 135-140.	2.6	50
46	Anomalous Wetting Layer at the Au(111) Surface. Journal of Physical Chemistry Letters, 2011, 2, 2582-2586.	4.6	50
47	Water Adsorption on Native and Hydrogenated Diamond (001) Surfaces. Journal of Physical Chemistry C, 2010, 114, 7045-7053.	3.1	47
48	Light-Induced Field Enhancement in Nanoscale Systems from First-Principles: The Case of Polyacenes. ACS Photonics, 2014, 1, 1049-1058.	6.6	47
49	Surface-Enhanced Fluorescence within a Metal Nanoparticle Array: The Role of Solvent and Plasmon Couplings. Journal of Physical Chemistry C, 2011, 115, 5450-5460.	3.1	46
50	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.	2.5	43
51	Solvent Effects on trans/gauche Conformational Equilibria of Substituted Chloroethanes:â€‰a Polarizable Continuum Model Study. Journal of Physical Chemistry A, 2001, 105, 10807-10815.	2.5	42
52	First-principles density-functional theory calculations of electron-transfer rates in azurin dimers. Journal of Chemical Physics, 2006, 124, 064501.	3.0	42
53	Proteinâ€"surface interactions: challenging experiments and computations. Journal of Molecular Recognition, 2010, 23, 259-262.	2.1	41
54	Surface Packing Determines the Redox Potential Shift of Cytochrome c Adsorbed on Gold. Journal of the American Chemical Society, 2014, 136, 12929-12937.	13.7	39

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55	Electronic and vibrational dynamic solvent effects on Raman spectra. Journal of Chemical Physics, 2001, 115, 5531-5535.	3.0	38
56	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.	2.6	38
57	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.	2.8	38
58	A Density Functional Theory Study of Cytosine on Au(111). Journal of Physical Chemistry C, 2012, 116, 21366-21373.	3.1	38
59	Can small hydrophobic gold nanoparticles inhibit Î²₂-microglobulin fibrillation?. Nanoscale, 2014, 6, 7903-7911.	5.6	37
60	Lifetimes of electronic excited states of a molecule close to a metal surface. Journal of Chemical Physics, 2003, 118, 6481-6494.	3.0	36
61	Enthalpyâ€“Entropy Tuning in the Adsorption of Nucleobases at the Au(111) Surface. Journal of Chemical Theory and Computation, 2014, 10, 1707-1716.	5.3	36
62	Tip-Enhanced Infrared Difference-Nanospectroscopy of the Proton Pump Activity of Bacteriorhodopsin in Single Purple Membrane Patches. Nano Letters, 2019, 19, 3104-3114.	9.1	36
63	Plasmon-Controlled Light-Harvesting: Design Rules for Biohybrid Devices via Multiscale Modeling. Nano Letters, 2013, 13, 4475-4484.	9.1	35
64	A few key residues determine the high redox potential shift in azurin mutants. Organic and Biomolecular Chemistry, 2015, 13, 11003-11013.	2.8	35
65	The interaction of peptides and proteins with nanostructures surfaces: a challenge for nanoscience. Current Opinion in Colloid and Interface Science, 2019, 41, 86-94.	7.4	35
66	Real-Time Description of the Electronic Dynamics for a Molecule Close to a Plasmonic Nanoparticle. Journal of Physical Chemistry C, 2016, 120, 28774-28781.	3.1	34
67	Interaction of Nucleic Acid Bases with the Au(111) Surface. Journal of Chemical Theory and Computation, 2013, 9, 4552-4561.	5.3	33
68	Peptide Synthesis of Gold Nanoparticles: The Early Steps of Gold Reduction Investigated by Density Functional Theory. Nano Letters, 2011, 11, 1313-1318.	9.1	32
69	Optical Excitations and Field Enhancement in Short Graphene Nanoribbons. Journal of Physical Chemistry Letters, 2012, 3, 924-929.	4.6	32
70	Distance-Based Configurational Entropy of Proteins from Molecular Dynamics Simulations. PLoS ONE, 2015, 10, e0132356.	2.5	32
71	Strong Coupling between Localized Surface Plasmons and Molecules by Coupled Cluster Theory. Nano Letters, 2021, 21, 6664-6670.	9.1	32
72	Citrate stabilized gold nanoparticles interfere with amyloid fibril formation: D76N and Î”N6 Î²2-microglobulin variants. Nanoscale, 2018, 10, 4793-4806.	5.6	30

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73	Interaction with a Gold Surface Reshapes the Free Energy Landscape of Alanine Dipeptide. Journal of Physical Chemistry C, 2014, 118, 11357-11364.	3.1	29
74	Water-Mediated Electron Transfer between Protein Redox Centers. Journal of Physical Chemistry B, 2007, 111, 3774-3781.	2.6	27
75	Single-Molecule Folding Mechanism of an EF-Hand Neuronal Calcium Sensor. Structure, 2013, 21, 1812-1821.	3.3	27
76	Hybrid theoretical models for molecular nanoplasmonics. Journal of Chemical Physics, 2020, 153, 200901.	3.0	27
77	Citrate-stabilized gold nanoparticles hinder fibrillogenesis of a pathological variant of Î²₂-microglobulin. Nanoscale, 2017, 9, 3941-3951.	5.6	26
78	Size dependence of the electron-hole recombination rates in semiconductor quantum dots. Physical Review B, 2003, 67, .	3.2	25
79	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.	2.6	25
80	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.	4.6	25
81	Fibrillation-prone conformations of the amyloid-Î²-42 peptide at the gold/water interface. Nanoscale, 2017, 9, 2279-2290.	5.6	25
82	A classical picture of subnanometer junctions: an atomistic Drude approach to nanoplasmonics. Nanoscale, 2019, 11, 6004-6015.	5.6	25
83	Photochemistry in the strong coupling regime: A trajectory surface hopping scheme. Journal of Computational Chemistry, 2020, 41, 2033-2044.	3.3	25
84	Insight on Chirality Encoding from Small Thiolated Molecule to Plasmonic Au@Ag and Au@Au Nanoparticles. ACS Nano, 2022, 16, 1089-1101.	14.6	25
85	Role of the electronic properties of azurin active site in the electron-transfer process. International Journal of Quantum Chemistry, 2005, 102, 328-342.	2.0	24
86	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.	5.3	24
87	The cavity electromagnetic field within the polarizable continuum model of solvation. Journal of Chemical Physics, 2014, 140, 164114.	3.0	23
88	Plasmonic Resonances of Metal Nanoparticles: Atomistic vs. Continuum Approaches. Frontiers in Chemistry, 2020, 8, 340.	3.6	23
89	Electronic Coupling Between Azurin and Gold at Different Protein/Substrate Orientations. Small, 2007, 3, 1431-1437.	10.0	22
90	van der Waals effects at molecule-metal interfaces. Physical Review B, 2014, 90, .	3.2	22

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91	Nonplasmonic Metal Particles as Excitation Energy Transfer Acceptors: an Unexpected Efficiency Revealed by Quantum Mechanics. Journal of Physical Chemistry C, 2009, 113, 16364-16370.	3.1	21
92	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.	3.1	21
93	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.	2.8	20
94	Interplay between Intra- and Intermolecular Charge Transfer in the Optical Excitations of J-Aggregates. Journal of Physical Chemistry C, 2019, 123, 6831-6838.	3.1	20
95	Self-Assembly of Mono- And Bidentate Oligoarylene Thiols onto Polycrystalline Au. Langmuir, 2013, 29, 13198-13208.	3.5	19
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.	2.5	19
97	Direct monitoring of opto-mechanical switching of self-assembled monolayer films containing the azobenzene group. Beilstein Journal of Nanotechnology, 2011, 2, 834-844.	2.8	18
98	First-principle-based MD description of azobenzene molecular rods. Theoretical Chemistry Accounts, 2012, 131, 1.	1.4	18
99	Can we control the electronic energy transfer in molecular dyads through metal nanoparticles? A QM/continuum investigation. Physical Chemistry Chemical Physics, 2013, 15, 3294.	2.8	18
100	Extending the essential dynamics analysis to investigate molecular properties: application to the redox potential of proteins. Physical Chemistry Chemical Physics, 2016, 18, 18450-18459.	2.8	18
101	Probing quantum coherence in ultrafast molecular processes: An ab initio approach to open quantum systems. Journal of Chemical Physics, 2018, 148, 204112.	3.0	18
102	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.	2.8	17
103	Full configuration interaction studies of phonon and photon transition rates in semiconductor quantum dots. Molecular Physics, 2002, 100, 911-918.	1.7	16
104	Water Effects on Electron Transfer in Azurin Dimers. Journal of Physical Chemistry B, 2006, 110, 23796-23800.	2.6	16
105	A Theoretical Study of the Electrochemical Gate Effect in an STM-Based Biomolecular Transistor. IEEE Nanotechnology Magazine, 2007, 6, 561-570.	2.0	16
106	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.	3.1	16
107	Exciton Transfer of Azobenzene Derivatives in Self-Assembled Monolayers. Journal of Physical Chemistry C, 2013, 117, 25026-25041.	3.1	16
108	Modeling opto-electronic properties of a dye molecule in proximity of a semiconductor nanoparticle. Journal of Chemical Physics, 2013, 139, 024105.	3.0	16

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109	Solid-State Effects on the Optical Excitation of Pushâ€“Pull Molecular J-Aggregates by First-Principles Simulations. ACS Omega, 2018, 3, 10481-10486.	3.5	15
110	Effects of Ligand Binding on the Energy Landscape of Acyl-CoA-Binding Protein. Biophysical Journal, 2020, 119, 1821-1832.	0.5	15
111	Simulating Plasmon Resonances of Gold Nanoparticles with Bipyramidal Shapes by Boundary Element Methods. Journal of Chemical Theory and Computation, 2020, 16, 3807-3815.	5.3	15
112	A new algorithm for rigid body molecular dynamics. Chemical Physics, 2006, 328, 259-268.	1.9	14
113	Self-consistent quantum mechanical model for the description of excitation energy transfers in molecules at interfaces. Journal of Chemical Physics, 2006, 125, 054710.	3.0	14
114	Quenching of the Photoisomerization of Azobenzene Self-Assembled Monolayers by the Metal Substrate. Journal of Physical Chemistry C, 2014, 118, 25906-25917.	3.1	14
115	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.	3.0	14
116	Role of coherence in the plasmonic control of molecular absorption. Journal of Chemical Physics, 2019, 151, 044703.	3.0	14
117	An open quantum system theory for polarizable continuum models. Journal of Chemical Physics, 2020, 152, 174114.	3.0	14
118	Prediction of Solvent Effects on Vibrational Absorption Intensities and Raman Activities in Solution within the Polarizable Continuum Model:â€‰ A Study on Pushâ^'Pull Molecules. Journal of Physical Chemistry A, 2003, 107, 10261-10271.	2.5	13
119	Second-order MÃ¸Ã¸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.	1.4	13
120	Retention of nativelike conformation by proteins embedded in high external electric fields. Journal of Chemical Physics, 2005, 122, 181102.	3.0	13
121	Structural Properties of Azobenzene Self-Assembled Monolayers by Atomistic Simulations. Langmuir, 2013, 29, 10505-10512.	3.5	13
122	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.	3.0	13
123	Quantum optimal control with quantum computers: A hybrid algorithm featuring machine learning optimization. Physical Review A, 2021, 103, .	2.5	13
124	Molecular Dynamics Simulations of a Catalytic Multivalent Peptideâ€“Nanoparticle Complex. International Journal of Molecular Sciences, 2021, 22, 3624.	4.1	13
125	Visualizing electron correlation by means of ab initio scanning tunneling spectroscopy images of single molecules. Journal of Chemical Physics, 2011, 134, 024104.	3.0	12
126	The Structure of Neuronal Calcium Sensor-1 in Solution Revealed by Molecular Dynamics Simulations. PLoS ONE, 2013, 8, e74383.	2.5	12

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127	Water splitting of hydrogen chemisorbed in graphene oxide dynamically evolves into a graphane lattice. Carbon, 2019, 153, 234-241.	10.3	12
128	Selective switching of multiple plexcitons in colloidal materials: directing the energy flow at the nanoscale. Nanoscale, 2021, 13, 6005-6015.	5.6	12
129	Stabilization energies of charged multiexciton complexes calculated at configuration interaction level. Physica E: Low-Dimensional Systems and Nanostructures, 2003, 18, 436-442.	2.7	11
130	A dynamical approach to non-adiabatic electron transfers at the bio-inorganic interface. Physical Chemistry Chemical Physics, 2016, 18, 10538-10549.	2.8	11
131	LayerPCM: An implicit scheme for dielectric screening from layered substrates. Journal of Chemical Physics, 2021, 154, 224114.	3.0	11
132	Modeling solvation effects in real-space and real-time within density functional approaches. Journal of Chemical Physics, 2015, 143, 144111.	3.0	10
133	Non-linear optical response by functionalized gold nanospheres: identifying design principles to maximize the molecular photo-release. Nanoscale, 2015, 7, 13345-13357.	5.6	10
134	Low-Resolution Models for the Interaction Dynamics of Coated Gold Nanoparticles with Î²2-microglobulin. International Journal of Molecular Sciences, 2019, 20, 3866.	4.1	10
135	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.	4.6	10
136	Infrared linear dichroism in stretched films: Quantum mechanical approach within the polarizable continuum model. International Journal of Quantum Chemistry, 2005, 104, 716-726.	2.0	9
137	Low-lying electronic excitations and optical absorption spectra of the black dye sensitizer: a first-principles study. Theoretical Chemistry Accounts, 2012, 131, 1.	1.4	9
138	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.	7.8	9
139	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.	7.8	9
140	Work Function Changes of Azo-Derivatives Adsorbed on a Gold Surface. Journal of Physical Chemistry C, 2014, 118, 26033-26040.	3.1	9
141	First-Principle Molecular Dynamics of Sliding Diamond Surfaces: Tribochemical Reactions with Water and Load Effects. Journal of Low Temperature Physics, 2016, 185, 174-182.	1.4	9
142	Adsorption Mechanisms of Nucleobases on the Hydrated Au(111) Surface. Langmuir, 2018, 34, 14749-14756.	3.5	9
143	Role of Organic Ligands Orientation on the Geometrical and Optical Properties of Au₂₅(SCH₃)₁₈⁰. Journal of Physical Chemistry A, 2018, 122, 6864-6872.	2.5	9
144	Shaping excitons in light-harvesting proteins through nanoplasmonics. Chemical Science, 2018, 9, 6219-6227.	7.4	9

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145	Quantifying the Plasmonic Character of Optical Excitations in a Molecular J-Aggregate. Journal of Chemical Theory and Computation, 2019, 15, 3197-3203.	5.3	9
146	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.	5.3	9
147	Atomistic simulations of gold surface functionalization for nanoscale biosensors applications. Nanotechnology, 2021, 32, 095702.	2.6	9
148	Proteins and Peptides at Gold Surfaces: Insights from Atomistic Simulations. ACS Symposium Series, 2012, , 229-250.	0.5	8
149	Dynamical Treatment of Charge Transfer through Duplex Nucleic Acids Containing Modified Adenines. ACS Nano, 2013, 7, 9396-9406.	14.6	8
150	Computational Strategies for Protein-Surface and Protein-Nanoparticle Interactions. Journal of Self-Assembly and Molecular Electronics (SAME), 0, , 1-26.	0.0	8
151	Quantum optimal control theory for solvated systems. Journal of Chemical Physics, 2019, 151, 194109.	3.0	8
152	Investigating ultrafast two-pulse experiments on single DNQDI fluorophores: a stochastic quantum approach. Physical Chemistry Chemical Physics, 2020, 22, 16734-16746.	2.8	8
153	Proline isomerization effects in the amyloidogenic protein Î²₂-microglobulin. Physical Chemistry Chemical Physics, 2021, 23, 356-367.	2.8	8
154	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.	5.3	8
155	High affinity protein surface binding through co-engineering of nanoparticles and proteins. Nanoscale, 2022, 14, 2411-2418.	5.6	7
156	Atomistic Simulations of Functionalized Nano-Materials for Biosensors Applications. International Journal of Molecular Sciences, 2022, 23, 1484.	4.1	7
157	Engineering the Aggregation of Dyes on Ligand-Shell Protected Gold Nanoparticles to Promote Plexcitons Formation. Nanomaterials, 2022, 12, 1180.	4.1	7
158	Azurin for Biomolecular Electronics: a Reliability Study. Japanese Journal of Applied Physics, 2005, 44, 6864-6866.	1.5	6
159	Reactivity of the ZnS(101Ì…0) Surface to Small Organic Ligands by Density Functional Theory. Journal of Physical Chemistry C, 2013, 117, 16034-16041.	3.1	6
160	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.	3.1	6
161	Excitation energy-transfer in functionalized nanoparticles: Going beyond the FÃ¶rster approach. Journal of Chemical Physics, 2016, 144, 074101.	3.0	6
162	Atomistic insight into the aggregation of [Au₂₅(SR)₁₈]^q nanoclusters. Nanoscale Advances, 2020, 2, 2842-2852.	4.6	6

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163	Study of the Rate-Determining Step of Rh Catalyzed CO2 Reduction: Insight on the Hydrogen Assisted Molecular Dissociation. Catalysts, 2021, 11, 538.	3.5	6
164	Lanthanide Ions Sensitization by Small Noble Metal Nanoclusters. ACS Photonics, 2021, 8, 1364-1376.	6.6	6
165	Exploring AuRh Nanoalloys: A Computational Perspective on the Formation and Physical Properties. ChemPhysChem, 2022, 23, .	2.1	6
166	Role of metal-nanostructure features on tip-enhanced photoluminescence of single molecules. Journal of Chemical Physics, 2021, 155, 214304.	3.0	6
167	Computational approach to study electron-transfer proteins: Azurin for bio-molecular devices. Computer Physics Communications, 2005, 169, 9-13.	7.5	5
168	Studying SERS from Metal Nanoparticles and Nanoparticles Aggregates with Continuum Models. , 2006, , 105-123.		5
169	Formation energy of dangling bonds on hydrogenated diamond surfaces: A first-principles study. Physical Review B, 2012, 85, .	3.2	5
170	How the Dynamics of the Metal-Binding Loop Region Controls the Acid Transition in Cupredoxins. Biochemistry, 2013, 52, 7397-7404.	2.5	5
171	Simulation of Proteinâ€“Surface Interactions by a Coarse-Grained Method. BioNanoScience, 2013, 3, 12-20.	3.5	5
172	Wettability of Azobenzene Self-Assembled Monolayers. Langmuir, 2014, 30, 4415-4421.	3.5	5
173	Correlation Effects in Scanning Tunneling Microscopy Images of Molecules Revealed by Quantum Monte Carlo. Journal of Chemical Theory and Computation, 2016, 12, 5339-5349.	5.3	5
174	Adsorption and Motion of Single Molecular Motors on TiO2(110). Journal of Physical Chemistry C, 2020, 124, 24776-24785.	3.1	5
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