Rosa Di Felice

List of Publications by Year
in descending order

83	3,539	147566	143772
papers	citations	31 h-index	57 g-index

87	87	87	4744
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	DNAshape: a method for the high-throughput prediction of DNA structural features on a genomic scale. Nucleic Acids Research, 2013, 41, W56-W62.	6.5	265
2	Long-range charge transport in single G-quadruplex DNA molecules. Nature Nanotechnology, 2014, 9, 1040-1046.	15.6	218
3	DFT Study of Cysteine Adsorption on Au(111). Journal of Physical Chemistry B, 2003, 107, 1151-1156.	1.2	200
4	Absorption Properties of Metalâ€“Semiconductor Hybrid Nanoparticles. ACS Nano, 2011, 5, 4712-4719.	7.3	199
5	Adsorption modes of cysteine on Au(111): Thiolate, amino-thiolate, disulfide. Journal of Chemical Physics, 2004, 120, 4906-4914.	1.2	190
6	Electronic structure of single DNA molecules resolved by transverse scanning tunnelling spectroscopy. Nature Materials, 2008, 7, 68-74.	13.3	140
7	Mixing of Electronic States in Pentacene Adsorption on Copper. Physical Review Letters, 2007, 99, 046802.	2.9	132
8	Quantum annealing versus classical machine learning applied to a simplified computational biology problem. Npj Quantum Information, 2018, 4, .	2.8	126
9	A TDDFT Study of the Excited States of DNA Bases and Their Assemblies. Journal of Physical Chemistry B, 2006, 110, 7129-7138.	1.2	112
10	Highly conductive self-assembled nanoribbons of coordination polymers. Nature Nanotechnology, 2010, 5, 110-115.	15.6	94
11	Polarizability of G4-DNA Observed by Electrostatic Force Microscopy Measurements. Nano Letters, 2007, 7, 981-986.	4.5	83
12	Ordered (3 Ã— 4) High-Density Phase of Methylthiolate on Au(111). Journal of Physical Chemistry B, 2004, 108, 16-20.	1.2	79
13	Ab initiostudy of model guanine assemblies: The role ofÏ€â^Ï€coupling and band transport. Physical Review B, 2001, 65, .	1.1	78
14	Control of DNA minor groove width and Fis protein binding by the purine 2-amino group. Nucleic Acids Research, 2013, 41, 6750-6760.	6.5	74
15	Simulation of Peptideâ€“Surface Recognition. Journal of Physical Chemistry Letters, 2011, 2, 1510-1519.	2.1	67
16	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
17	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
18	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

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19	Ab Initio Optical Absorption Spectra of Size-Expanded xDNA Base Assemblies. Journal of Physical Chemistry B, 2007, 111, 14012-14021.	1.2	49
20	Stability and Migration of Metal Ions in G4-Wires by Molecular Dynamics Simulations. Journal of Physical Chemistry B, 2006, 110, 26337-26348.	1.2	47
21	Towards a gauge invariant method for molecular chiroptical properties in TDDFT. Physical Chemistry Chemical Physics, 2009, 11, 4481.	1.3	46
22	Conductive Nanostructures of MMX Chains. Advanced Functional Materials, 2010, 20, 1451-1457.	7.8	45
23	Metallicity in Individual MMX Chains. Journal of the American Chemical Society, 2008, 130, 5552-5562.	6.6	41
24	Proteinâ€“surface interactions: challenging experiments and computations. Journal of Molecular Recognition, 2010, 23, 259-262.	1.1	41
25	Porphyrin Intercalation in G4-DNA Quadruplexes by Molecular Dynamics Simulations. Journal of Physical Chemistry B, 2009, 113, 13152-13160.	1.2	40
26	Electrical Conductivity in Platinum-Dimer Columns. Inorganic Chemistry, 2008, 47, 9736-9738.	1.9	39
27	A Density Functional Theory Study of Cytosine on Au(111). Journal of Physical Chemistry C, 2012, 116, 21366-21373.	1.5	38
28	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
29	Electronic Properties of Metal-Modified DNA Base Pairs. Journal of Physical Chemistry B, 2008, 112, 14281-14290.	1.2	35
30	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
31	On the Magnetic Alignment of Metal Ions in a DNA-Mimic Double Helix. Journal of Physical Chemistry B, 2005, 109, 15345-15348.	1.2	33
32	Interaction of Nucleic Acid Bases with the Au(111) Surface. Journal of Chemical Theory and Computation, 2013, 9, 4552-4561.	2.3	33
33	Dielectric Functions of Semiconductor Nanoparticles from the Optical Absorption Spectrum: The Case of CdSe and CdS. Journal of Physical Chemistry C, 2010, 114, 3776-3780.	1.5	31
34	Strain-Dependence of the Electronic Properties in Periodic Quadruple Helical G4-Wires. Journal of Physical Chemistry B, 2005, 109, 22301-22307.	1.2	28
35	Electron Channels in Biomolecular Nanowires. Journal of Physical Chemistry B, 2004, 108, 2509-2515.	1.2	27
36	Water-Mediated Electron Transfer between Protein Redox Centers. Journal of Physical Chemistry B, 2007, 111, 3774-3781.	1.2	27

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37	Scanning Tunneling Spectroscopy of Single DNA Molecules. ACS Nano, 2009, 3, 1651-1656.	7.3	27
38	Single-Molecule Folding Mechanism of an EF-Hand Neuronal Calcium Sensor. Structure, 2013, 21, 1812-1821.	1.6	27
39	Symmetry lowering of pentacene molecular states interacting with a Cu surface. Physical Review B, 2007, 76, .	1.1	26
40	Nature of the Interaction between Natural and Size-Expanded Guanine with Gold Clusters: A Density Functional Theory Study. Journal of Physical Chemistry C, 2012, 116, 24954-24961.	1.5	25
41	Fibrillation-prone conformations of the amyloid-Î²-42 peptide at the gold/water interface. Nanoscale, 2017, 9, 2279-2290.	2.8	25
42	Charge Transfer between [4Fe4S] Proteins and DNA Is Unidirectional: Implications for Biomolecular Signaling. CheM, 2019, 5, 122-137.	5.8	25
43	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
44	CRISPRâ€“Cas9 Mediated DNA Unwinding Detected Using Site-Directed Spin Labeling. ACS Chemical Biology, 2017, 12, 1489-1493.	1.6	24
45	Electronic Coupling Between Azurin and Gold at Different Protein/Substrate Orientations. Small, 2007, 3, 1431-1437.	5.2	22
46	van der Waals effects at molecule-metal interfaces. Physical Review B, 2014, 90, .	1.1	22
47	Atomic and Electronic Structure at Au/CdSe Interfaces. ACS Nano, 2008, 2, 2225-2236.	7.3	21
48	Combined effects of metal complexation and size expansion in the electronic structure of DNA base pairs. Journal of Chemical Physics, 2011, 134, 205102.	1.2	21
49	Electronic Structure of G4-DNA by Scanning Tunneling Spectroscopy. Journal of Physical Chemistry C, 2010, 114, 22079-22084.	1.5	20
50	Optical Properties of Triplex DNA from Time-Dependent Density Functional Theory. Journal of Physical Chemistry B, 2012, 116, 10693-10702.	1.2	20
51	Energy Gap Reduction in DNA by Complexation with Metal Ions. Advanced Materials, 2011, 23, 4290-4294.	11.1	19
52	Electrical Behaviour of Heterobimetallic [MMâ€²(EtCS₂)₄] (MMâ€²=NiPd, NiPt, PdPt) and MMâ€²Xâ€Chain Polymers [PtM(EtCS₂)₄I] (M=Ni, Pd). Chemistry - A European Journal, 2012, 18, 15476-15484.	1.7	19
53	Conformations of Human Telomeric G-Quadruplex Studied Using a Nucleotide-Independent Nitroxide Label. Biochemistry, 2016, 55, 360-372.	1.2	19
54	Optical spectra of nitride quantum dots: Quantum confinement and electronâ€“hole coupling. Applied Physics Letters, 1999, 75, 3449-3451.	1.5	17

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55	Fingerprints of Bonding Motifs in DNA Duplexes of Adenine and Thymine Revealed from Circular Dichroism: Synchrotron Radiation Experiments and TDDFT Calculations. Journal of Physical Chemistry B, 2009, 113, 9614-9619.	1.2	17
56	Landscape of DNA binding signatures of myocyte enhancer factor-2B reveals a unique interplay of base and shape readout. Nucleic Acids Research, 2020, 48, 8529-8544.	6.5	17
57	Water Effects on Electron Transfer in Azurin Dimers. Journal of Physical Chemistry B, 2006, 110, 23796-23800.	1.2	16
58	Ab initio Study of the Structural, Tautomeric, Pairing, and Electronic Properties of Seleno-Derivatives of Thymine. Journal of Physical Chemistry B, 2009, 113, 14465-14472.	1.2	15
59	Electron delocalization at the hybrid aromatic-thiolâˆ•Cu(100)interface. Physical Review B, 2004, 70, .	1.1	13
60	The Structure of Neuronal Calcium Sensor-1 in Solution Revealed by Molecular Dynamics Simulations. PLoS ONE, 2013, 8, e74383.	1.1	12
61	Is the G-Quadruplex an Effective Nanoconductor for Ions?. Journal of Physical Chemistry B, 2014, 118, 864-872.	1.2	12
62	The RNA Polymerase Î± Subunit Recognizes the DNA Shape of the Upstream Promoter Element. Biochemistry, 2020, 59, 4523-4532.	1.2	12
63	Effects of G-Quadruplex Topology on Electronic Transfer Integrals. Nanomaterials, 2016, 6, 184.	1.9	10
64	Protein-Mutation-Induced Conformational Changes of the DNA and Nuclease Domain in CRISPR/Cas9 Systems by Molecular Dynamics Simulations. Journal of Physical Chemistry B, 2020, 124, 2168-2179.	1.2	10
65	Adsorption Mechanisms of Nucleobases on the Hydrated Au(111) Surface. Langmuir, 2018, 34, 14749-14756.	1.6	9
66	Dynamical Treatment of Charge Transfer through Duplex Nucleic Acids Containing Modified Adenines. ACS Nano, 2013, 7, 9396-9406.	7.3	8
67	Effects of Structural Dynamics on Charge Carrier Transfer in B-DNA: A Combined MD and RT-TDDFT Study. Journal of Physical Chemistry B, 2021, 125, 3986-4003.	1.2	8
68	Interaction of DNA Bases with Gold Substrates. Journal of Self-Assembly and Molecular Electronics (SAME), 0, , .	0.0	7
69	Investigating the Chinese postman problem on a quantum annealer. Quantum Machine Intelligence, 2021, 3, 1.	2.7	7
70	Azurin for Biomolecular Electronics: a Reliability Study. Japanese Journal of Applied Physics, 2005, 44, 6864-6866.	0.8	6
71	Surface functionalization through adsorption of organic molecules. Journal of Physics Condensed Matter, 2007, 19, 305018.	0.7	6
72	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

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73	Computational approach to study electron-transfer proteins: Azurin for bio-molecular devices. Computer Physics Communications, 2005, 169, 9-13.	3.0	5
74	LCAO Electronic Structure of Nucleic Acid Bases and Other Heterocycles and Transfer Integrals in B-DNA, Including Structural Variability. Materials, 2021, 14, 4930.	1.3	4
75	DNA-Based Nanoelectronics. , 2008, , 141-185.		4
76	Electronic Structure Calculations for Nanomolecular Systems. , 2006, , 77-116.		3
77	Charge Transfer Rates at a Bioâ€“Inorganic Interface. Journal of Physical Chemistry C, 2014, 118, 18820-18828.	1.5	3
78	Theoretical analysis of the optical spectra of InxGa1âˆ’xN quantum dots in InyGa1âˆ’yN layers. Physica E: Low-Dimensional Systems and Nanostructures, 2000, 7, 934-938.	1.3	2
79	Electronic structure of DNA derivatives and mimics by density functional theory. , 2006, , 485-507.		2
80	Optical Enhancement in Heteroleptic Ru(II) Polypyridyl Complexes Using Electron-Donor Ancillary Ligands. Journal of Physical Chemistry C, 2014, 118, 8747-8755.	1.5	2
81	Molecular Simulations have Boosted Knowledge of CRISPR/Cas9: A Review. Journal of Self-Assembly and Molecular Electronics (SAME), 2019, 7, 45-72.	0.0	2
82	DNA-Based Nanoelectronics. Nanostructure Science and Technology, 2009, , 43-79.	0.1	2
83	DNA from First Principles. , 2016, , 800-819.		0