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List of Publications by Year in descending order

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87
papers

1,792
citations

257450

24
h-index

315739

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all docs

89
docs citations

89
times ranked

2621
citing authors

#	ARTICLE	IF	CITATIONS
1	Membrane Environment Modulates Ligand-Binding Propensity of P2Y12 Receptor. <i>Pharmaceutics</i> , 2021, 13, 524.	4.5	4
2	Influence of Substrate Hydrophilicity on Structural Properties of Supported Lipid Systems on Graphene, Graphene Oxides, and Silica. <i>Journal of Physical Chemistry B</i> , 2021, 125, 8060-8074.	2.6	1
3	Albumin-driven disassembly of lipidic nanoparticles: the specific case of the squalene-adenosine nanodrug. <i>Nanoscale</i> , 2020, 12, 2793-2809.	5.6	9
4	Lipoproteins LDL versus HDL as nanocarriers to target either cancer cells or macrophages. <i>JCI Insight</i> , 2020, 5, .	5.0	5
5	Stacking as a Key Property for Creating Nanoparticles with Tunable Shape: The Case of Squalenoyl-Doxorubicin. <i>ACS Nano</i> , 2019, 13, 12870-12879.	14.6	10
6	Fate of cisplatin and its main hydrolysed forms in the presence of thiolates: a comprehensive computational and experimental study. <i>Metallomics</i> , 2019, 11, 833-844.	2.4	8
7	The asymmetry of plasma membranes and their cholesterol content influence the uptake of cisplatin. <i>Scientific Reports</i> , 2019, 9, 5627.	3.3	95
8	Curvature increases permeability of the plasma membrane for ions, water and the anti-cancer drugs cisplatin and gemcitabine. <i>Scientific Reports</i> , 2019, 9, 17214.	3.3	34
9	Low-Density Lipoproteins and Human Serum Albumin as Carriers of Squalenoylated Drugs: Insights from Molecular Simulations. <i>Molecular Pharmaceutics</i> , 2018, 15, 585-591.	4.6	29
10	Squalene versus cholesterol: Which is the best nanocarrier for the delivery to cells of the anticancer drug gemcitabine?. <i>Comptes Rendus Chimie</i> , 2018, 21, 974-986.	0.5	10
11	Conjugation of squalene to gemcitabine as unique approach exploiting endogenous lipoproteins for drug delivery. <i>Nature Communications</i> , 2017, 8, 15678.	12.8	86
12	Structures of single, double and triple layers of lipids adsorbed on graphene: Insights from all-atom molecular dynamics simulations. <i>Carbon</i> , 2017, 118, 358-369.	10.3	9
13	The influence of curvature on the properties of the plasma membrane. Insights from atomistic molecular dynamics simulations. <i>Scientific Reports</i> , 2017, 7, 16078.	3.3	67
14	Selective Inhibition of STAT3 with Respect to STAT1: Insights from Molecular Dynamics and Ensemble Docking Simulations. <i>Journal of Chemical Information and Modeling</i> , 2016, 56, 1588-1596.	5.4	17
15	Interaction of C ₆₀ fullerenes with asymmetric and curved lipid membranes: a molecular dynamics study. <i>Physical Chemistry Chemical Physics</i> , 2016, 18, 278-284.	2.8	18
16	A molecular dynamics study of catestatin docked on nicotinic acetylcholine receptors to identify amino acids potentially involved in the binding of chromogranin A fragments. <i>Physical Chemistry Chemical Physics</i> , 2015, 17, 17454-17460.	2.8	7
17	Theoretical insights into the mechanism of redox switch in heat shock protein Hsp33. <i>Journal of Biological Inorganic Chemistry</i> , 2015, 20, 555-562.	2.6	15
18	A theoretical study of the unfolding pathway of reduced Human serum albumin. <i>Journal of Molecular Modeling</i> , 2015, 21, 106.	1.8	2

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19	Empirical force field for cisplatin based on quantum dynamics data: case study of new parameterization scheme for coordination compounds. <i>Journal of Molecular Modeling</i> , 2015, 21, 268.	1.8	20
20	Novel aminotetrazole derivatives as selective STAT3 non-peptide inhibitors. <i>European Journal of Medicinal Chemistry</i> , 2015, 103, 163-174.	5.5	32
21	A principal component analysis of the dynamics of subdomains and binding sites in human serum albumin. <i>Biopolymers</i> , 2014, 101, 561-572.	2.4	18
22	Determination of mean and Gaussian curvatures of highly curved asymmetric lipid bilayers: the case study of the influence of cholesterol on the membrane shape. <i>Physical Chemistry Chemical Physics</i> , 2014, 16, 17052.	2.8	26
23	Insertion kinetics of small nucleotides through single walled carbon nanotube. <i>Journal of Biotechnology</i> , 2013, 164, 13-18.	3.8	4
24	Oxidation reactivity of zinc-cysteine clusters in metallothionein. <i>Journal of Biological Inorganic Chemistry</i> , 2013, 18, 333-342.	2.6	13
25	Efficiency of the monofunctionalized C60fullerenes as membrane targeting agents studied by all-atom molecular dynamics simulations. <i>Molecular Membrane Biology</i> , 2013, 30, 338-345.	2.0	5
26	How do functionalized carbon nanotubes land on, bind to and pierce through model and plasma membranes. <i>Nanoscale</i> , 2013, 5, 10242.	5.6	61
27	Enhanced potassium selectivity in a bioinspired solid nanopore. <i>Physical Chemistry Chemical Physics</i> , 2013, 15, 19601.	2.8	5
28	Will C-Laurdan Dethrone Laurdan in Fluorescent Solvent Relaxation Techniques for Lipid Membrane Studies?. <i>Langmuir</i> , 2013, 29, 1174-1182.	3.5	35
29	Controlling potassium selectivity and proton blocking in a hybrid biological/solid-state polymer nanoporous membrane. <i>Nanoscale</i> , 2013, 5, 3961.	5.6	24
30	How long a functionalized carbon nanotube can passively penetrate a lipid membrane. <i>Carbon</i> , 2012, 50, 5301-5308.	10.3	26
31	About the structural role of disulfide bridges in serum albumins: Evidence from protein simulated unfolding. <i>Biopolymers</i> , 2012, 97, 889-898.	2.4	37
32	Insertion of Short Amino-Functionalized Single-Walled Carbon Nanotubes into Phospholipid Bilayer Occurs by Passive Diffusion. <i>PLoS ONE</i> , 2012, 7, e40703.	2.5	67
33	Oxidation of Zinc-Thiolate Complexes of Biological Interest by Hydrogen Peroxide: A Theoretical Study. <i>Inorganic Chemistry</i> , 2011, 50, 5407-5416.	4.0	25
34	Stability of the gramicidin-A channel structure in view of nanofiltration: a computational and experimental study. <i>Soft Matter</i> , 2011, 7, 10651.	2.7	6
35	Uptake and Translocation Mechanisms of Cationic Amino Derivatives Functionalized on Pristine C60 by Lipid Membranes: A Molecular Dynamics Simulation Study. <i>ACS Nano</i> , 2011, 5, 8571-8578.	14.6	36
36	New Bioinspired Membrane Made of a Biological Ion Channel Confined into the Cylindrical Nanopore of a Solid-State Polymer.. <i>Nano Letters</i> , 2011, 11, 712-716.	9.1	51

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37	Formation of one-dimensional ordered alloy at step edges: An atomistic study of the (2 $\sqrt{3}$ -1) Ni/Pt alloy on the Pt(997) surface. <i>Surface Science</i> , 2011, 605, 917-922.	1.9	17
38	Scaling of submonolayer island sizes in Ag growth on stepped Pt surfaces. <i>Surface Science</i> , 2010, 604, 1576-1583.	1.9	9
39	CHARACTERIZATION OF SURFACE DEFECTS THROUGH THE MODIFICATION OF THE INFRARED PROFILE OF ADMOLECULES: APPLICATION TO CO MOLECULES ADSORBED ON (100) MgO AND NaCl SURFACES. <i>Surface Review and Letters</i> , 2010, 17, 431-436.	1.1	0
40	Numerical studies of the membrane fluorescent dyes dynamics in ground and excited states. <i>Biochimica Et Biophysica Acta - Biomembranes</i> , 2010, 1798, 1724-1734.	2.6	42
41	Affinity of C ₆₀ Neat Fullerenes with Membrane Proteins: A Computational Study on Potassium Channels. <i>ACS Nano</i> , 2010, 4, 4158-4164.	14.6	63
42	Growth of perfect and smooth Ag and Co monatomic wires on Pt vicinal surfaces: A kinetic Monte Carlo study. <i>Surface Science</i> , 2009, 603, 22-26.	1.9	13
43	Probing defect species on real surfaces from the analysis of the spectral profile of admolecules. <i>Surface Science</i> , 2009, 603, 887-894.	1.9	0
44	Determination of the charge profile in the KcsA selectivity filter using ab initio calculations and molecular dynamics simulations. <i>Physical Chemistry Chemical Physics</i> , 2009, 11, 8606.	2.8	9
45	Is the mobility of the pore walls and water molecules in the selectivity filter of KcsA channel functionally important?. <i>Physical Chemistry Chemical Physics</i> , 2008, 10, 2249.	2.8	4
46	Conditions for organized nanoring growth using kinetic Monte Carlo simulations. <i>Physical Review B</i> , 2008, 77, .	3.2	3
47	Model for thermal desorption of hydrogen atoms from a graphite surface based on kinetic Monte Carlo simulations. <i>Physical Review B</i> , 2008, 77, .	3.2	22
48	First stages of epitaxial growth in the presence of an extended defect: Kinetic Monte Carlo simulations versus rate equation study on a vicinal surface. <i>Physical Review B</i> , 2007, 76, .	3.2	3
49	Insight into the origins of the barrier-less knock-on conduction in the KcsA channel: molecular dynamics simulations and ab initio calculations. <i>Physical Chemistry Chemical Physics</i> , 2007, 9, 1219.	2.8	12
50	A Stable Room-Temperature Molecular Assembly of Zwitterionic Organic Dipoles Guided by a Si(111)-7 \times 7 Template Effect. <i>Angewandte Chemie - International Edition</i> , 2007, 46, 9287-9290.	13.8	32
51	Ion conductance vs. pore gating and selectivity in KcsA channel: Modeling achievements and perspectives. <i>Journal of Molecular Modeling</i> , 2007, 13, 699-713.	1.8	23
52	Dielectric constant of electrolyte solutions confined in a charged nanofiltration membrane. <i>Desalination</i> , 2006, 200, 125-126.	8.2	10
53	Determination of the single wall carbon nanotube opening ratio by means of rare gas adsorption. <i>Chemical Physics Letters</i> , 2006, 423, 183-186.	2.6	8
54	Direct growth of the multi-walled carbon nanotubes as a tool to detect ammonia at room temperature. <i>Chemical Physics Letters</i> , 2006, 433, 175-181.	2.6	55

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55	Negative ion resonance of a molecule adsorbed on a metal surface covered with a rare gas monolayer. <i>Surface Science</i> , 2006, 600, 803-814.	1.9	6
56	First-principles investigation of Co wires at Pt(111) step-edges. <i>Surface Science</i> , 2006, 600, 4301-4304.	1.9	9
57	Incidence of partial charges on ion selectivity in potassium channels. <i>Journal of Chemical Physics</i> , 2006, 124, 044703.	3.0	23
58	Relaxation effects on the magnetism of decorated step edges:Co ⁺ Pt(664). <i>Physical Review B</i> , 2006, 73, .	3.2	28
59	Zip gating of the KcsA channel studied by targeted molecular dynamics. <i>Chemical Physics Letters</i> , 2005, 407, 199-204.	2.6	4
60	Targeted molecular dynamics of an open-state KcsA channel. <i>Journal of Chemical Physics</i> , 2005, 122, 134707.	3.0	34
61	Alignment of single-wall carbon nanotubes by inclusion of dipolar wires. <i>Physical Review B</i> , 2005, 72, .	3.2	4
62	Role of water molecules in the KcsA protein channel by molecular dynamics calculations. <i>Physical Chemistry Chemical Physics</i> , 2005, 7, 4138.	2.8	12
63	Orientalional ordering in physisorbed molecular layers induced by surface geometry and confinement. <i>International Journal of Quantum Chemistry</i> , 2004, 99, 735-742.	2.0	1
64	Grating formation in step flow heterogeneous growth and wavelength selection induced by confinement. <i>Surface Science</i> , 2004, 553, L68-L74.	1.9	7
65	Ab initio investigation of the atomic charges in the KcsA channel selectivity filter. <i>Chemical Physics Letters</i> , 2004, 397, 510-515.	2.6	23
66	Comparative study of ab initio and tight-binding electronic structure calculations applied to platinum surfaces. <i>Physical Review B</i> , 2004, 70, .	3.2	40
67	Molecular selectivity due to adsorption properties in nanotubes. <i>Physical Review B</i> , 2004, 69, .	3.2	80
68	Molecular dynamics study of the KcsA channel at 2.0-Å... resolution: stability and concerted motions within the pore. <i>Biochimica Et Biophysica Acta - Biomembranes</i> , 2004, 1661, 26-39.	2.6	45
69	Ab initio study of the influence of conformation on partial charge distribution of dioctadecylamine. <i>Chemical Physics Letters</i> , 2003, 380, 424-434.	2.6	1
70	Atomic diffusion inside a STM junction: simulations by kinetic Monte Carlo coupled to tunneling current calculations. <i>Surface Science</i> , 2003, 523, 267-278.	1.9	8
71	Image states on a free-electron metal surface covered by an atomically thin insulator layer. <i>Surface Science</i> , 2003, 528, 78-83.	1.9	15
72	Improvement of nanowire distributions with a STM tip: a kinetic Monte Carlo approach. <i>Surface Science</i> , 2003, 532-535, 531-535.	1.9	0

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73	Quantum-well resonances and image states in the Ar/Cu(110) system. Surface Science, 2003, 540, 457-473.	1.9	21
74	Selective adsorption and structure formation of N ₂ on the nanostructured Cu-CuO stripe phase. Physical Review B, 2002, 66, .	3.2	15
75	Ordering of nitrogen molecules on the nanostructured Cu(110)/Cu(110)-(2 \times 1)O stripe phase. Surface Science, 2001, 482-485, 1379-1384.	1.9	2
76	Reply to "Comment on "Effect of the structural anisotropy and lateral strain on the surface phonons of monolayer xenon on Cu(110)" Physical Review B, 2001, 64, .	3.2	2
77	Growth of composition-modulated Ag/Co wires on Pt(997). Physical Review B, 2001, 64, .	3.2	31
78	Confinement effects on the growth of adsorbates: Interpretation of the formation of monoatomic Ag wires on Pt(997). Physical Review B, 2000, 61, 16154-16162.	3.2	33
79	Influence of step geometry and orientation on the growth of adsorbates. Surface Science, 2000, 454-456, 106-111.	1.9	2
80	Resonant electron scattering by N ₂ molecules on Ag(110): study of the orientational ordering of the N ₂ physisorbed layers. Surface Science, 2000, 465, 138-148.	1.9	5
81	Adsorption and structure of N ₂ on Pt(111). Surface Science, 2000, 444, 163-179.	1.9	20
82	Effect of the diffusion anisotropy on the nucleation and growth of xenon on Cu(110). Surface Science, 2000, 446, L113-L119.	1.9	14
83	Structure of N ₂ adlayers on the highly corrugated Cu(110)-(2 \times 1)O surface. Surface Science, 1999, 423, 175-188.	1.9	8
84	Dynamics of confined Xe monolayers adsorbed on the Pt(997) vicinal surface. Surface Science, 1998, 400, 176-188.	1.9	5
85	Characterization of the Cu(110)-(2 \times 1)O reconstruction by means of molecular adsorption. Physical Review B, 1998, 58, 9998-10002.	3.2	22
86	N ₂ monolayer and bilayer adsorbed on Ag(110) at 15 K: Structure and orientational ordering. Physical Review B, 1998, 58, 4111-4119.	3.2	16
87	Structure of Xe adsorbed on the highly corrugated Cu(110)-(2 \times 1)O surface. Physical Review B, 1998, 57, 13149-13157.	3.2	13