Oscar Bertran

List of Publications by Year
in descending order

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Version: 2024-02-01

53 papers	841 citations	586496 16 h-index	620720 26 g-index
53 all docs	53 docs citations	53 times ranked	1171 citing authors

#	Article	IF	Citations
1	Computer simulations on oxidative stress-induced reactions in SARS-CoV-2 spike glycoprotein: a multi-scale approach. Molecular Diversity, 2022, , 1.	2.1	0
2	Temperature effect on the SARS-CoV-2: A molecular dynamics study of the spike homotrimeric glycoprotein. Computational and Structural Biotechnology Journal, 2021, 19, 1848-1862.	1.9	16
3	A model study on controlling dealloying corrosion attack by lateral modification of surfactant inhibitors. Npj Materials Degradation, 2021, 5, .	2.6	8
4	A revised solution for a sphere rolling in a vertical loop. European Journal of Physics, 2021, 42, 015008.	0.3	5
5	Molecular dynamics simulations on self-healing behavior of ionene polymer-based nanostructured hydrogels. Polymer, 2020, 211, 123072.	1.8	10
6	Analysis of nitrogen fixation by a catalyst capable of transforming N2, CO2 and CH4 into amino acids under mild reactions conditions. Applied Catalysis A: General, 2020, 596, 117526.	2.2	9
7	Main-chain scission of individual macromolecules induced by solvent swelling. Chemical Science, 2019, 10, 6125-6139.	3.7	13
8	Hydroxyapatite with Permanent Electrical Polarization: Preparation, Characterization, and Response against Inorganic Adsorbates. ChemPhysChem, 2018, 19, 1746-1755.	1.0	21
9	Cationic ionene as an n-dopant agent of poly(3,4-ethylenedioxythiophene). Physical Chemistry Chemical Physics, 2018, 20, 9855-9864.	1.3	9
10	2. Close Contacts at the interface: Experimental-computational synergies for solving complexity problems. , 2018, , 53-80.		0
11	Close contacts at the interface: Experimental-computational synergies for solving complexity problems. ChemistrySelect, 2018, 3, .	0.7	1
12	Isomeric cationic ionenes as n-dopant agents of poly(3,4-ethylenedioxythiophene) for <i>in situ</i> gelation. Soft Matter, 2018, 14, 6374-6385.	1.2	8
13	Aromatic ionene topology and counterion-tuned gelation of acidic aqueous solutions. Soft Matter, 2017, 13, 3031-3041.	1.2	14
14	Solvatochromism of dye-labeled dendronized polymers of generation numbers 1â€“4: comparison to dendrimers. Chemical Science, 2016, 7, 4644-4652.	3.7	9
15	Effects of hydroxyapatite (0001) Ca²⁺/Mg²⁺substitution on adsorbed<scp>d</scp>-ribose ring puckering. RSC Advances, 2016, 6, 69634-69640.	1.7	3
16	Dissolving Hydroxyolite: A DNA Molecule into Its Hydroxyapatite Mold. Chemistry - A European Journal, 2016, 22, 6631-6636.	1.7	13
17	Surviving Mass Extinctions through Biomineralized DNA. Chemistry - A European Journal, 2015, 21, 18892-18898.	1.7	6
18	Synergistic Approach to Elucidate the Incorporation of Magnesium Ions into Hydroxyapatite. Chemistry - A European Journal, 2015, 21, 2537-2546.	1.7	24

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19	An experimental-computer modeling study of inorganic phosphates surface adsorption on hydroxyapatite particles. Dalton Transactions, 2015, 44, 9980-9991.	1.6	15
20	Modeling Nanosized Single Molecule Objects: Dendronized Polymers Adsorbed onto Mica. Journal of Physical Chemistry C, 2015, 119, 3746-3753.	1.5	11
21	Internal organization of macromonomers and dendronized polymers based on thiophene dendrons. Soft Matter, 2015, 11, 1116-1126.	1.2	5
22	DNA adsorbed on hydroxyapatite surfaces. Journal of Materials Chemistry B, 2014, 2, 6953-6966.	2.9	41
23	Interactions in dendronized polymers: intramolecular dominates intermolecular. Soft Matter, 2014, 10, 1032.	1.2	16
24	Mineralization of DNA into nanoparticles of hydroxyapatite. Dalton Transactions, 2014, 43, 317-327.	1.6	39
25	Influence of the Temperature on the Proton Transport in Poly(styrene-co-divinylbenzene) Membranes from Molecular Dynamics Simulations. Journal of Physical Chemistry C, 2014, 118, 17643-17654.	1.5	5
26	Electroactive polymers for the detection of morphine. Journal of Polymer Research, 2014, 21, 1.	1.2	6
27	Restricted Puckering of Mineralized RNA-Like Riboses. Journal of Physical Chemistry B, 2014, 118, 5075-5081.	1.2	5
28	Modeling biominerals formed by apatites and DNA. Biointerphases, 2013, 8, 10.	0.6	28
29	Transport of hydronium ions inside poly(styrene-co-divinyl benzene) cation exchange membranes. Journal of Membrane Science, 2013, 428, 393-402.	4.1	16
30	Atomistic organization and characterization of tube-like assemblies comprising peptideâ€“polymer conjugates: computer simulation studies. Faraday Discussions, 2013, 166, 59.	1.6	13
31	Computer simulation of dendronized polymers: organization and characterization at the atomistic level. RSC Advances, 2013, 3, 126-140.	1.7	26
32	Computer Simulation of Fifth Generation Dendronized Polymers: Impact of Charge on Internal Organization. Journal of Physical Chemistry B, 2013, 117, 6007-6017.	1.2	20
33	Linear Viscoelastic Response of Dendronized Polymers. Macromolecules, 2012, 45, 8813-8823.	2.2	29
34	On the modeling of aggregates of an optically active regioregular polythiophene. Physical Chemistry Chemical Physics, 2012, 14, 1881.	1.3	9
35	Properties of Oligothiophene Dendrimers as a Function of Molecular Architecture and Generation Number. ChemPhysChem, 2012, 13, 1354-1362.	1.0	4
36	Thermodynamic and stereochemical aspects of the polymerizability of glycolide and lactide. Theoretical Chemistry Accounts, 2012, 131, 1.	0.5	7

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37	Ultrathin Films of Polypyrrole Derivatives for Dopamine Detection. Journal of Physical Chemistry C, 2011, 115, 14933-14941.	1.5	57
38	Electronic properties of poly(thiophene-3-methyl acetate). Journal of Polymer Research, 2011, 18, 1509-1517.	1.2	17
39	Parameterization of the torsional potential for calix[4]areneâ€substituted poly(thiophene)s. Journal of Computational Chemistry, 2010, 31, 1741-1751.	1.5	6
40	Field-Induced Transport in Sulfonated Poly(styrene-<i>co</i>-divinylbenzene) Membranes. Macromolecules, 2010, 43, 10521-10527.	2.2	14
41	Incorporation of deMon2k as a new parallel quantum mechanical code for the PUPIL system. Journal of Computational Chemistry, 2010, 31, 2669-2676.	1.5	4
42	Modeling the Structural and Electronic Properties of an Optically Active Regioregular Polythiophene. Journal of Physical Chemistry C, 2010, 114, 11074-11080.	1.5	11
43	Poly(2-thiophen-3-yl-malonic acid), a Polythiophene with Two Carboxylic Acids Per Repeating Unit. Journal of Physical Chemistry B, 2010, 114, 6281-6290.	1.2	33
44	Characterization and properties of a polythiophene with a malonic acid dimethyl ester side group. European Polymer Journal, 2009, 45, 2211-2221.	2.6	25
45	Controlled Isomerization of a Light-Driven Molecular Motor: A Theoretical Study. Journal of Physical Chemistry C, 2009, 113, 3574-3580.	1.5	25
46	Structural and Electronic Properties of Poly(thiaheterohelicene)s. Journal of Physical Chemistry B, 2009, 113, 15196-15203.	1.2	15
47	Thermodynamic Control of the Polymerizability of Five-, Six-, and Seven-Membered Lactones. Journal of Organic Chemistry, 2009, 74, 6237-6244.	1.7	74
48	Structural and electronic properties of poly(3-thiophen-3-yl-acrylic acid). Polymer, 2008, 49, 1972-1980.	1.8	12
49	Correlation between symmetry breaker position and the preferences of conformationally constrained homopeptides: A molecular dynamics investigation. Biopolymers, 2008, 90, 695-706.	1.2	15
50	Cross-linking in polypyrrole and poly(N-methylpyrrole): Comparative experimental and theoretical studies. Polymer, 2008, 49, 1066-1075.	1.8	29
51	Modelling organic molecular crystals by hybrid quantum mechanical/molecular mechanical embedding. Chemical Physics Letters, 2008, 457, 154-158.	1.2	15
52	Hydrogen-Bonding Interactions in 2-Thiophen-3-ylmalonic Acid. Journal of Physical Chemistry A, 2008, 112, 10650-10656.	1.1	7
53	On the structural and electronic properties of poly(3-thiophen-3-yl-acrylic acid methyl ester). Polymer, 2007, 48, 6955-6964.	1.8	18