Maria Fyta

List of Publications by Year
in descending order

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83 papers	1,769 citations	361045 20 h-index	301761 39 g-index
85 all docs	85 docs citations	85 times ranked	2165 citing authors

#	Article	IF	Citations
1	Confined Ruâ€catalysts in a Twoâ€phase Heptane/Ionic Liquid Solution: Modeling Aspects. ChemCatChem, 2021, 13, 739-746.	1.8	2
2	Dynamics and Solvent Effects in Functionalized DNA Sensing Nanogaps. , 2021, , 155-166.		1
3	Deep learning for nanopore ionic current blockades. Journal of Chemical Physics, 2021, 154, 044111.	1.2	21
4	Energetic Arguments on the Microstructural Analysis in Ionic Liquids. Advanced Theory and Simulations, 2021, 4, 2100114.	1.3	2
5	Simple Classification of RNA Sequences of Respiratory-Related Coronaviruses. ACS Omega, 2021, 6, 20158-20165.	1.6	1
6	Impact of COVID-19 on Electricity Demand: Deriving Minimum States of System Health for Studies on Resilience. Data, 2021, 6, 76.	1.2	0
7	Adsorption of azide-functionalized thiol linkers on zinc oxide surfaces. RSC Advances, 2021, 11, 5466-5478.	1.7	7
8	Lateral MoS₂ Heterostructure for Sensing Small Gas Molecules. ACS Applied Electronic Materials, 2020, 2, 74-83.	2.0	13
9	Lithium adsorption on 2D transition metal dichalcogenides: towards a descriptor for machine learned materials design. Journal of Materials Chemistry A, 2020, 8, 23511-23518.	5.2	20
10	Electrically sensing Hachimoji DNA nucleotides through a hybrid graphene/h-BN nanopore. Nanoscale, 2020, 12, 18289-18295.	2.8	24
11	Functionalized Nanogap for DNA Readâ€Out: Nucleotide Rotation and Currentâ€Voltage Curves. ChemPhysChem, 2020, 21, 2068-2074.	1.0	5
12	Domain-size effect on the electronic properties of two-dimensional MoS2/WS2. Physical Review B, 2020, 101, .	1.1	1
13	2D MoS₂ nanopores: ionic current blockade height for clustering DNA events. 2D Materials, 2019, 6, 045011.	2.0	8
14	In silico Complexes of Amino Acids and Diamondoids. ChemPhysChem, 2019, 20, 2166-2170.	1.0	2
15	High flux and CO2-resistance of La0.6Ca0.4Co1â€“Fe O3â^' oxygen-transporting membranes. Journal of Membrane Science, 2019, 590, 117082.	4.1	25
16	Probing DNA nucleobases with diamond (111) surfaces. Journal of Physics Communications, 2019, 3, 095007.	0.5	0
17	The influence of a solvent on the electronic transport across diamondoid-functionalized biosensing electrodes. Nanoscale, 2019, 11, 14216-14225.	2.8	11
18	Aqueous Mixtures of Room-Temperature Ionic Liquids: Entropy-Driven Accumulation of Water Molecules at Interfaces. Journal of Physical Chemistry C, 2019, 123, 13795-13803.	1.5	29

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19	Enhancing the optical detection of mutants from healthy DNA with diamondoids. Journal of Materials Chemistry B, 2019, 7, 3424-3430.	2.9	6
20	Hybrid 2D nanodevices (graphene/h-BN): selecting NO_x gas through the device interface. Journal of Materials Chemistry A, 2019, 7, 8905-8911.	5.2	29
21	Vacancy defect centers in diamond: influence of surface termination. European Physical Journal: Special Topics, 2019, 227, 1591-1601.	1.2	4
22	Diamondoid-functionalized nanogaps: from small molecules to electronic biosensing. European Physical Journal: Special Topics, 2019, 227, 1681-1692.	1.2	4
23	Electronic features of vacancy, nitrogen, and phosphorus defects in nanodiamonds. Electronic Structure, 2019, 1, 025002.	1.0	4
24	Interplay of structural, electronic, and transport features in copper alloys. Journal of Alloys and Compounds, 2019, 777, 619-626.	2.8	6
25	Hybrids made of defective nanodiamonds interacting with DNA nucleobases. Nanotechnology, 2019, 30, 065601.	1.3	1
26	Optical Properties of Single- and Double-Functionalized Small Diamondoids. Journal of Physical Chemistry A, 2018, 122, 3583-3593.	1.1	10
27	Two-Dimensional Metallic/Semiconducting MoS₂ under Biaxial Strain. ACS Applied Nano Materials, 2018, 1, 5562-5570.	2.4	11
28	Optoelectronic Properties of Diamondoid-DNA Complexes. ACS Applied Bio Materials, 2018, 1, 59-69.	2.3	11
29	Coarse-Grained Double-Stranded RNA Model from Quantum-Mechanical Calculations. Journal of Physical Chemistry B, 2018, 122, 7915-7928.	1.2	10
30	Vibrational states of nano-confined water molecules in beryl investigated by first-principles calculations and optical experiments. Physical Chemistry Chemical Physics, 2017, 19, 30740-30748.	1.3	16
31	Insights into the detection of mutations and epigenetic markers using diamondoid-functionalized sensors. RSC Advances, 2017, 7, 43064-43072.	1.7	7
32	The properties of residual water molecules in ionic liquids: a comparison between direct and inverse Kirkwoodâ€“Buff approaches. Physical Chemistry Chemical Physics, 2017, 19, 18924-18937.	1.3	35
33	Electrokinetic Lattice Boltzmann Solver Coupled to Molecular Dynamics: Application to Polymer Translocation. Langmuir, 2017, 33, 11635-11645.	1.6	10
34	Carbene-mediated self-assembly of diamondoids on metal surfaces. Nanoscale, 2016, 8, 8966-8975.	2.8	20
35	Diamondoid-functionalized gold nanogaps as sensors for natural, mutated, and epigenetically modified DNA nucleotides. Nanoscale, 2016, 8, 10105-10112.	2.8	33
36	Complexes of carbene-functionalized diamondoids and metal atoms: Electronic properties. Journal of Organometallic Chemistry, 2016, 815-816, 8-15.	0.8	5

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37	Benchmark investigation of diamondoid-functionalized electrodes for nanopore DNA sequencing. Nanotechnology, 2016, 27, 414002.	1.3	12
38	Electronic Transport along Hybrid MoS₂ Monolayers. Journal of Physical Chemistry C, 2016, 120, 23389-23396.	1.5	14
39	Binding energies of nucleobase complexes: Relevance to homology recognition of DNA. Physical Review E, 2016, 93, 062410.	0.8	3
40	Diamondoid-based molecular junctions: a computational study. Nanotechnology, 2016, 27, 485207.	1.3	1
41	Towards double-functionalized small diamondoids: selective electronic band-gap tuning. Nanotechnology, 2015, 26, 035701.	1.3	13
42	Threading DNA through nanopores for biosensing applications. Journal of Physics Condensed Matter, 2015, 27, 273101.	0.7	22
43	Typeâ€Dependent Identification of DNA Nucleobases by Using Diamondoids. ChemPhysChem, 2014, 15, 3466-3475.	1.0	3
44	Diamondoids as DNA methylation and mutation probes. Europhysics Letters, 2014, 108, 17005.	0.7	6
45	Promoting the assembly of carbon onions: An atomistic approach. Physica Status Solidi (A) Applications and Materials Science, 2014, 211, 277-287.	0.8	4
46	The role of a diamondoid as a hydrogen donor or acceptor in probing DNA nucleobases. European Physical Journal E, 2014, 37, 95.	0.7	9
47	Stable boron nitride diamondoids as nanoscale materials. Nanotechnology, 2014, 25, 365601.	1.3	7
48	Chemically modified diamondoids as biosensors for DNA. Nanoscale, 2014, 6, 4225-4232.	2.8	20
49	Nitrogen-Vacancy Centers and Dopants in Ultrathin Diamond Films: Electronic Structure. Journal of Physical Chemistry C, 2013, 117, 21376-21381.	1.5	19
50	Force fields for divalent cations based on single-ion and ion-pair properties. Journal of Chemical Physics, 2013, 138, 024505.	1.2	118
51	Ionic force field optimization based on single-ion and ion-pair solvation properties: Going beyond standard mixing rules. Journal of Chemical Physics, 2012, 136, 124103.	1.2	129
52	Ab initio determination of coarse-grained interactions in double-stranded DNA. Journal of Chemical Physics, 2012, 137, 105102.	1.2	33
53	Computer simulations of nanostructured carbon under tensile load: Electronic structure and optical gap. Diamond and Related Materials, 2012, 23, 50-53.	1.8	4
54	Disorder and optical gaps in strained dense amorphous carbon and diamond nanocomposites. Journal of Physics Condensed Matter, 2012, 24, 205502.	0.7	3

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55	Structural and technical details of the Kirkwood-Buff integrals from the optimization of ionic force fields: focus on fluorides. European Physical Journal E, 2012, 35, 1-12.	0.7	7
56	Carbon-based nanostructured composite films: Elastic, mechanical and optoelectronic properties derived from computer simulations. Surface and Coatings Technology, 2011, 206, 696-702.	2.2	6
57	Translocation of biomolecules through solidâ€state nanopores: Theory meets experiments. Journal of Polymer Science, Part B: Polymer Physics, 2011, 49, 985-1011.	2.4	46
58	Large scale simulation of quantum-mechanical molecular dynamics for nano-polycrystalline diamond. Journal of Physics: Conference Series, 2010, 215, 012118.	0.3	0
59	Ionic force field optimization based on single-ion and ion-pair solvation properties. Journal of Chemical Physics, 2010, 132, 024911.	1.2	71
60	Quantized biopolymer translocation through nanopores: Departure from simple scaling. Physical Review E, 2009, 79, 030901.	0.8	8
61	MUPHY: A parallel MUlti PHYsics/scale code for high performance bio-fluidic simulations. Computer Physics Communications, 2009, 180, 1495-1502.	3.0	109
62	Ion-Specificity: From Solvation Thermodynamics to Molecular Simulations and Back. , 2009, , 231-265.		6
63	Numerical simulation of conformational variability in biopolymer translocation through wide nanopores. Journal of Statistical Mechanics: Theory and Experiment, 2009, 2009, P06009.	0.9	6
64	Ab initiosupercell calculations on nitrogen-vacancy center in diamond: Electronic structure and hyperfine tensors. Physical Review B, 2008, 77, .	1.1	238
65	Multiscale Simulation of Nanobiological Flows. Computing in Science and Engineering, 2008, 10, 10-19.	1.2	19
66	Quantized Current Blockade and Hydrodynamic Correlations in Biopolymer Translocation through Nanopores: Evidence from Multiscale Simulations. Nano Letters, 2008, 8, 1115-1119.	4.5	30
67	MUPHY: A parallel high performance MUlti PHYsics/Scale code. Parallel and Distributed Processing Symposium (IPDPS), Proceedings of the International Conference on, 2008, , .	1.0	2
68	Hydrodynamic correlations in the translocation of a biopolymer through a nanopore: Theory and multiscale simulations. Physical Review E, 2008, 78, 036704.	0.8	83
69	Parallel Multiscale Modeling of Biopolymer Dynamics with Hydrodynamic Correlations. International Journal for Multiscale Computational Engineering, 2008, 6, 25-37.	0.8	8
70	EXPLORING DNA TRANSLOCATION THROUGH A NANOPORE VIA A MULTISCALE LATTICE-BOLTZMANN MOLECULAR-DYNAMICS METHODOLOGY. International Journal of Modern Physics C, 2007, 18, 685-692.	0.8	13
71	Structure, elastic properties and strength of amorphous and nanocomposite carbon. Diamond and Related Materials, 2007, 16, 1835-1840.	1.8	22
72	Atomic and electronic structure of crystallineâ€“amorphous carbon interfaces. Diamond and Related Materials, 2007, 16, 1875-1881.	1.8	21

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73	Probing the sp2 dependence of elastic moduli in ultrahard diamond films. Diamond and Related Materials, 2007, 16, 1643-1647.	1.8	13
74	Simulations on the elastic response of amorphous and nanocomposite carbon. Diamond and Related Materials, 2007, 16, 1676-1681.	1.8	2
75	Multiscale model of electronic behavior and localization in stretched dry DNA. Journal of Materials Science, 2007, 42, 8894-8903.	1.7	5
76	Multiscale Modeling of Biopolymer Translocation Through a Nanopore. Lecture Notes in Computer Science, 2007, , 786-793.	1.0	0
77	Multiscale Coupling of Molecular Dynamics and Hydrodynamics: Application to DNA Translocation through a Nanopore. Multiscale Modeling and Simulation, 2006, 5, 1156-1173.	0.6	88
78	Insights into the Fracture Mechanisms and Strength of Amorphous and Nanocomposite Carbon. Physical Review Letters, 2006, 96, 185503.	2.9	73
79	Structure, stability, and stress properties of amorphous and nanostructured carbon films. Thin Solid Films, 2005, 482, 56-62.	0.8	12
80	Computer Simulations of Carbon Nanostructures under Pressure. Fullerenes Nanotubes and Carbon Nanostructures, 2005, 13, 13-20.	1.0	2
81	Simulations of composite carbon films with nanotube inclusions. Applied Physics Letters, 2005, 86, 191916.	1.5	11
82	Energetics and stability of nanostructured amorphous carbon. Physical Review B, 2003, 67, .	1.1	35
83	Stress variations near surfaces in diamond-like amorphous carbon. Journal of Non-Crystalline Solids, 2000, 266-269, 760-764.	1.5	15