

# Maria Fyta

## List of Publications by Year in descending order

Source: <https://exaly.com/author-pdf/4993435/publications.pdf>

Version: 2024-02-01

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	<i>Ab initio</i> supercell calculations on nitrogen-vacancy center in diamond: Electronic structure and hyperfine tensors. <i>Physical Review B</i> , 2008, 77, .	1.1	238
2	Ionic force field optimization based on single-ion and ion-pair solvation properties: Going beyond standard mixing rules. <i>Journal of Chemical Physics</i> , 2012, 136, 124103.	1.2	129
3	Force fields for divalent cations based on single-ion and ion-pair properties. <i>Journal of Chemical Physics</i> , 2013, 138, 024505.	1.2	118
4	MUPHY: A parallel Multi PHYSics/scale code for high performance bio-fluidic simulations. <i>Computer Physics Communications</i> , 2009, 180, 1495-1502.	3.0	109
5	Multiscale Coupling of Molecular Dynamics and Hydrodynamics: Application to DNA Translocation through a Nanopore. <i>Multiscale Modeling and Simulation</i> , 2006, 5, 1156-1173.	0.6	88
6	Hydrodynamic correlations in the translocation of a biopolymer through a nanopore: Theory and multiscale simulations. <i>Physical Review E</i> , 2008, 78, 036704.	0.8	83
7	Insights into the Fracture Mechanisms and Strength of Amorphous and Nanocomposite Carbon. <i>Physical Review Letters</i> , 2006, 96, 185503.	2.9	73
8	Ionic force field optimization based on single-ion and ion-pair solvation properties. <i>Journal of Chemical Physics</i> , 2010, 132, 024911.	1.2	71
9	Translocation of biomolecules through solid-state nanopores: Theory meets experiments. <i>Journal of Polymer Science, Part B: Polymer Physics</i> , 2011, 49, 985-1011.	2.4	46
10	Energetics and stability of nanostructured amorphous carbon. <i>Physical Review B</i> , 2003, 67, .	1.1	35
11	The properties of residual water molecules in ionic liquids: a comparison between direct and inverse Kirkwood- <i>Buff</i> approaches. <i>Physical Chemistry Chemical Physics</i> , 2017, 19, 18924-18937.	1.3	35
12	<i>Ab initio</i> determination of coarse-grained interactions in double-stranded DNA. <i>Journal of Chemical Physics</i> , 2012, 137, 105102.	1.2	33
13	Diamondoid-functionalized gold nanogaps as sensors for natural, mutated, and epigenetically modified DNA nucleotides. <i>Nanoscale</i> , 2016, 8, 10105-10112.	2.8	33
14	Quantized Current Blockade and Hydrodynamic Correlations in Biopolymer Translocation through Nanopores: Evidence from Multiscale Simulations. <i>Nano Letters</i> , 2008, 8, 1115-1119.	4.5	30
15	Aqueous Mixtures of Room-Temperature Ionic Liquids: Entropy-Driven Accumulation of Water Molecules at Interfaces. <i>Journal of Physical Chemistry C</i> , 2019, 123, 13795-13803.	1.5	29
16	Hybrid 2D nanodevices (graphene/h-BN): selecting NO <sub>x</sub> gas through the device interface. <i>Journal of Materials Chemistry A</i> , 2019, 7, 8905-8911.	5.2	29
17	High flux and CO <sub>2</sub> -resistance of La <sub>0.6</sub> Ca <sub>0.4</sub> Co <sub>1</sub> Fe <sub>0.3</sub> oxygen-transporting membranes. <i>Journal of Membrane Science</i> , 2019, 590, 117082.	4.1	25
18	Electrically sensing Hachimoji DNA nucleotides through a hybrid graphene/h-BN nanopore. <i>Nanoscale</i> , 2020, 12, 18289-18295.	2.8	24

#	ARTICLE	IF	CITATIONS
19	Structure, elastic properties and strength of amorphous and nanocomposite carbon. <i>Diamond and Related Materials</i> , 2007, 16, 1835-1840.	1.8	22
20	Threading DNA through nanopores for biosensing applications. <i>Journal of Physics Condensed Matter</i> , 2015, 27, 273101.	0.7	22
21	Atomic and electronic structure of crystalline-amorphous carbon interfaces. <i>Diamond and Related Materials</i> , 2007, 16, 1875-1881.	1.8	21
22	Deep learning for nanopore ionic current blockades. <i>Journal of Chemical Physics</i> , 2021, 154, 044111.	1.2	21
23	Chemically modified diamondoids as biosensors for DNA. <i>Nanoscale</i> , 2014, 6, 4225-4232.	2.8	20
24	Carbene-mediated self-assembly of diamondoids on metal surfaces. <i>Nanoscale</i> , 2016, 8, 8966-8975.	2.8	20
25	Lithium adsorption on 2D transition metal dichalcogenides: towards a descriptor for machine learned materials design. <i>Journal of Materials Chemistry A</i> , 2020, 8, 23511-23518.	5.2	20
26	Multiscale Simulation of Nanobiological Flows. <i>Computing in Science and Engineering</i> , 2008, 10, 10-19.	1.2	19
27	Nitrogen-Vacancy Centers and Dopants in Ultrathin Diamond Films: Electronic Structure. <i>Journal of Physical Chemistry C</i> , 2013, 117, 21376-21381.	1.5	19
28	Vibrational states of nano-confined water molecules in beryl investigated by first-principles calculations and optical experiments. <i>Physical Chemistry Chemical Physics</i> , 2017, 19, 30740-30748.	1.3	16
29	Stress variations near surfaces in diamond-like amorphous carbon. <i>Journal of Non-Crystalline Solids</i> , 2000, 266-269, 760-764.	1.5	15
30	Electronic Transport along Hybrid MoS <sub>2</sub> Monolayers. <i>Journal of Physical Chemistry C</i> , 2016, 120, 23389-23396.	1.5	14
31	EXPLORING DNA TRANSLOCATION THROUGH A NANOPORE VIA A MULTISCALE LATTICE-BOLTZMANN MOLECULAR-DYNAMICS METHODOLOGY. <i>International Journal of Modern Physics C</i> , 2007, 18, 685-692.	0.8	13
32	Probing the sp <sup>2</sup> dependence of elastic moduli in ultrahard diamond films. <i>Diamond and Related Materials</i> , 2007, 16, 1643-1647.	1.8	13
33	Towards double-functionalized small diamondoids: selective electronic band-gap tuning. <i>Nanotechnology</i> , 2015, 26, 035701.	1.3	13
34	Lateral MoS <sub>2</sub> Heterostructure for Sensing Small Gas Molecules. <i>ACS Applied Electronic Materials</i> , 2020, 2, 74-83.	2.0	13
35	Structure, stability, and stress properties of amorphous and nanostructured carbon films. <i>Thin Solid Films</i> , 2005, 482, 56-62.	0.8	12
36	Benchmark investigation of diamondoid-functionalized electrodes for nanopore DNA sequencing. <i>Nanotechnology</i> , 2016, 27, 414002.	1.3	12

#	ARTICLE	IF	CITATIONS
37	Simulations of composite carbon films with nanotube inclusions. <i>Applied Physics Letters</i> , 2005, 86, 191916.	1.5	11
38	Two-Dimensional Metallic/Semiconducting MoS <sub>2</sub> under Biaxial Strain. <i>ACS Applied Nano Materials</i> , 2018, 1, 5562-5570.	2.4	11
39	Optoelectronic Properties of Diamondoid-DNA Complexes. <i>ACS Applied Bio Materials</i> , 2018, 1, 59-69.	2.3	11
40	The influence of a solvent on the electronic transport across diamondoid-functionalized biosensing electrodes. <i>Nanoscale</i> , 2019, 11, 14216-14225.	2.8	11
41	Electrokinetic Lattice Boltzmann Solver Coupled to Molecular Dynamics: Application to Polymer Translocation. <i>Langmuir</i> , 2017, 33, 11635-11645.	1.6	10
42	Optical Properties of Single- and Double-Functionalized Small Diamondoids. <i>Journal of Physical Chemistry A</i> , 2018, 122, 3583-3593.	1.1	10
43	Coarse-Grained Double-Stranded RNA Model from Quantum-Mechanical Calculations. <i>Journal of Physical Chemistry B</i> , 2018, 122, 7915-7928.	1.2	10
44	The role of a diamondoid as a hydrogen donor or acceptor in probing DNA nucleobases. <i>European Physical Journal E</i> , 2014, 37, 95.	0.7	9
45	Quantized biopolymer translocation through nanopores: Departure from simple scaling. <i>Physical Review E</i> , 2009, 79, 030901.	0.8	8
46	2D MoS <sub>2</sub> nanopores: ionic current blockade height for clustering DNA events. <i>2D Materials</i> , 2019, 6, 045011.	2.0	8
47	Parallel Multiscale Modeling of Biopolymer Dynamics with Hydrodynamic Correlations. <i>International Journal for Multiscale Computational Engineering</i> , 2008, 6, 25-37.	0.8	8
48	Structural and technical details of the Kirkwood-Buff integrals from the optimization of ionic force fields: focus on fluorides. <i>European Physical Journal E</i> , 2012, 35, 1-12.	0.7	7
49	Stable boron nitride diamondoids as nanoscale materials. <i>Nanotechnology</i> , 2014, 25, 365601.	1.3	7
50	Insights into the detection of mutations and epigenetic markers using diamondoid-functionalized sensors. <i>RSC Advances</i> , 2017, 7, 43064-43072.	1.7	7
51	Adsorption of azide-functionalized thiol linkers on zinc oxide surfaces. <i>RSC Advances</i> , 2021, 11, 5466-5478.	1.7	7
52	Ion-Specificity: From Solvation Thermodynamics to Molecular Simulations and Back. , 2009, , 231-265.		6
53	Numerical simulation of conformational variability in biopolymer translocation through wide nanopores. <i>Journal of Statistical Mechanics: Theory and Experiment</i> , 2009, 2009, P06009.	0.9	6
54	Carbon-based nanostructured composite films: Elastic, mechanical and optoelectronic properties derived from computer simulations. <i>Surface and Coatings Technology</i> , 2011, 206, 696-702.	2.2	6

#	ARTICLE	IF	CITATIONS
55	Diamondoids as DNA methylation and mutation probes. <i>Europhysics Letters</i> , 2014, 108, 17005.	0.7	6
56	Enhancing the optical detection of mutants from healthy DNA with diamondoids. <i>Journal of Materials Chemistry B</i> , 2019, 7, 3424-3430.	2.9	6
57	Interplay of structural, electronic, and transport features in copper alloys. <i>Journal of Alloys and Compounds</i> , 2019, 777, 619-626.	2.8	6
58	Multiscale model of electronic behavior and localization in stretched dry DNA. <i>Journal of Materials Science</i> , 2007, 42, 8894-8903.	1.7	5
59	Complexes of carbene-functionalized diamondoids and metal atoms: Electronic properties. <i>Journal of Organometallic Chemistry</i> , 2016, 815-816, 8-15.	0.8	5
60	Functionalized Nanogap for DNA Readout: Nucleotide Rotation and Current-Voltage Curves. <i>ChemPhysChem</i> , 2020, 21, 2068-2074.	1.0	5
61	Computer simulations of nanostructured carbon under tensile load: Electronic structure and optical gap. <i>Diamond and Related Materials</i> , 2012, 23, 50-53.	1.8	4
62	Promoting the assembly of carbon onions: An atomistic approach. <i>Physica Status Solidi (A) Applications and Materials Science</i> , 2014, 211, 277-287.	0.8	4
63	Vacancy defect centers in diamond: influence of surface termination. <i>European Physical Journal: Special Topics</i> , 2019, 227, 1591-1601.	1.2	4
64	Diamondoid-functionalized nanogaps: from small molecules to electronic biosensing. <i>European Physical Journal: Special Topics</i> , 2019, 227, 1681-1692.	1.2	4
65	Electronic features of vacancy, nitrogen, and phosphorus defects in nanodiamonds. <i>Electronic Structure</i> , 2019, 1, 025002.	1.0	4
66	Disorder and optical gaps in strained dense amorphous carbon and diamond nanocomposites. <i>Journal of Physics Condensed Matter</i> , 2012, 24, 205502.	0.7	3
67	Type-Dependent Identification of DNA Nucleobases by Using Diamondoids. <i>ChemPhysChem</i> , 2014, 15, 3466-3475.	1.0	3
68	Binding energies of nucleobase complexes: Relevance to homology recognition of DNA. <i>Physical Review E</i> , 2016, 93, 062410.	0.8	3
69	Computer Simulations of Carbon Nanostructures under Pressure. <i>Fullerenes Nanotubes and Carbon Nanostructures</i> , 2005, 13, 13-20.	1.0	2
70	Simulations on the elastic response of amorphous and nanocomposite carbon. <i>Diamond and Related Materials</i> , 2007, 16, 1676-1681.	1.8	2
71	MUPHY: A parallel high performance Multi PHYsics/Scale code. <i>Parallel and Distributed Processing Symposium (IPDPS), Proceedings of the International Conference on</i> , 2008, , .	1.0	2
72	In silico Complexes of Amino Acids and Diamondoids. <i>ChemPhysChem</i> , 2019, 20, 2166-2170.	1.0	2

#	ARTICLE	IF	CITATIONS
73	Confined Ru catalysts in a Two-phase Heptane/Ionic Liquid Solution: Modeling Aspects. ChemCatChem, 2021, 13, 739-746.	1.8	2
74	Energetic Arguments on the Microstructural Analysis in Ionic Liquids. Advanced Theory and Simulations, 2021, 4, 2100114.	1.3	2
75	Diamondoid-based molecular junctions: a computational study. Nanotechnology, 2016, 27, 485207.	1.3	1
76	Hybrids made of defective nanodiamonds interacting with DNA nucleobases. Nanotechnology, 2019, 30, 065601.	1.3	1
77	Domain-size effect on the electronic properties of two-dimensional MoS <sub>2</sub> /WS <sub>2</sub> . Physical Review B, 2020, 101, .	1.1	1
78	Dynamics and Solvent Effects in Functionalized DNA Sensing Nanogaps. , 2021, , 155-166.		1
79	Simple Classification of RNA Sequences of Respiratory-Related Coronaviruses. ACS Omega, 2021, 6, 20158-20165.	1.6	1
80	Large scale simulation of quantum-mechanical molecular dynamics for nano-polycrystalline diamond. Journal of Physics: Conference Series, 2010, 215, 012118.	0.3	0
81	Probing DNA nucleobases with diamond (111) surfaces. Journal of Physics Communications, 2019, 3, 095007.	0.5	0
82	Impact of COVID-19 on Electricity Demand: Deriving Minimum States of System Health for Studies on Resilience. Data, 2021, 6, 76.	1.2	0
83	Multiscale Modeling of Biopolymer Translocation Through a Nanopore. Lecture Notes in Computer Science, 2007, , 786-793.	1.0	0