Fabien Fp Picaud

List of Publications by Year
in descending order

106 papers	1,923 citations	293460 24 h-index	355658 38 g-index
110 all docs	110 docs citations	110 times ranked	2793 citing authors

#	Article	IF	Citations
1	Nanovectorization of Ivermectin to avoid overdose of drugs. Journal of Biomolecular Structure and Dynamics, 2023, 41, 4272-4285.	2.0	0
2	Molecular dynamics investigations of ionic conductance at the nanoscale: Role of the water model and geometric parameters. Journal of Molecular Liquids, 2022, 351, 118575.	2.3	9
3	From Behavior of Water on Hydrophobic Graphene Surfaces to Ultra-Confinement of Water in Carbon Nanotubes. Nanomaterials, 2021, 11, 306.	1.9	3
4	Breaking the Controversy of the Electropolymerization of Pyrrole Mechanisms by the Effective Screening Medium Quantum Charged Model Interface. Journal of Physical Chemistry A, 2021, 125, 1860-1869.	1.1	2
5	Confinement of the antitumoral drug cisplatin inside edge-functionalized carbon nanotubes and its release near lipid membrane. European Physical Journal D, 2021, 75, 1.	0.6	4
6	Impact of surface state on polyethylene glycol conformation confined inside a nanopore. Journal of Chemical Physics, 2021, 154, 104901.	1.2	6
7	A potential solution to avoid overdose of mixed drugs in the event of Covid-19: Nanomedicine at the heart of the Covid-19 pandemic. Journal of Molecular Graphics and Modelling, 2021, 104, 107834.	1.3	6
8	Detection of Amyloid-Î² Fibrils Using Track-Etched Nanopores: Effect of Geometry and Crowding. ACS Sensors, 2021, 6, 3733-3743.	4.0	20
9	Conformation of Polyethylene Glycol inside Confined Space: Simulation and Experimental Approaches. Nanomaterials, 2021, 11, 244.	1.9	9
10	Ionic Conductance of Carbon Nanotubes: Confronting Literature Data with Nanofluidic Theory. Journal of Physical Chemistry C, 2021, 125, 22943-22950.	1.5	6
11	The influence of hole networks on the adsorption-induced frequency shift of a perforated nanobeam using non-local elasticity theory. Journal of Physics and Chemistry of Solids, 2020, 136, 109201.	1.9	8
12	Ligand nanovectorization using graphene to target cellular death receptors of cancer cell. Proteins: Structure, Function and Bioinformatics, 2020, 88, 94-105.	1.5	5
13	Polynucleotide differentiation using hybrid solid-state nanopore functionalizing with Î±-hemolysin. Soft Matter, 2020, 16, 1002-1010.	1.2	8
14	First-principles study of the reaction mechanism governing the SNAr of the dimethylamine on 2-methoxy-5-nitrothiophenes. Theoretical Chemistry Accounts, 2020, 139, 1.	0.5	5
15	Behavior of anchor functionalized ZnPc molecules on a graphene nanoflake near membrane cell. Structural Chemistry, 2020, 31, 1935-1943.	1.0	1
16	Theoretical study of ciprofloxacin antibiotic trapping on graphene or boron nitride oxide nanoflakes. Journal of Molecular Modeling, 2020, 26, 135.	0.8	12
17	From Anodic Oxidation of Aliphatic Î±-Amino Acids to Polypeptides by Quantum Electrochemistry Approach: Beyond Millerâ€“Urey Experiments. Journal of the American Chemical Society, 2019, 141, 14230-14238.	6.6	7
18	Influence of nanotube section on carboplatin confinement. Journal of Molecular Modeling, 2019, 25, 72.	0.8	7

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19	Natural payload delivery of the doxorubicin anticancer drug from boron nitride oxide nanosheets. Applied Surface Science, 2019, 475, 666-675.	3.1	42
20	Unexpected ionic transport behavior in hydrophobic and uncharged conical nanopores. Faraday Discussions, 2018, 210, 69-85.	1.6	8
21	The encapsulation of the gemcitabine anticancer drug into grapheme nest: a theoretical study. Journal of Molecular Modeling, 2018, 24, 102.	0.8	16
22	N-glycosylation of mouse TRAIL-R and human TRAIL-R1 enhances TRAIL-induced death. Cell Death and Differentiation, 2017, 24, 500-510.	5.0	75
23	Boron Nitride Nanoporous Membranes with High Surface Charge by Atomic Layer Deposition. ACS Applied Materials & Interfaces, 2017, 9, 16669-16678.	4.0	83
24	TRAILâ€“NP hybrids for cancer therapy: a review. Nanoscale, 2017, 9, 5755-5768.	2.8	37
25	Discrimination of Polynucleotide Transport through a Highly Hydrophobic Uncharged Nanopore. Journal of Physical Chemistry C, 2017, 121, 7525-7532.	1.5	8
26	Simulations of a Graphene Nanoflake as a Nanovector To Improve ZnPc Phototherapy Toxicity: From Vacuum to Cell Membrane. ACS Applied Materials & Interfaces, 2017, 9, 37554-37562.	4.0	20
27	Controlling activation barrier by carbon nanotubes as nano-chemical reactors. Journal of Molecular Modeling, 2017, 23, 229.	0.8	2
28	Voltage-activated transport of ions through single-walled carbon nanotubes. Nanoscale, 2017, 9, 11976-11986.	2.8	32
29	Ab Initio Study of Azomethine Derivative Cancer Drug on Boron Nitride and Graphene Nanoflakes. Nanotechnology Nanomedicine & Nanobiotechnology, 2017, 4, 1-6.	0.1	5
30	Confined Nystatin Polyenes in Nanopore Induce Biologic Ionic Selectivity. Journal of Nanomaterials, 2016, 2016, 1-9.	1.5	2
31	Enhanced DR5 binding capacity of nanovectorized TRAIL compared to its cytotoxic version by affinity chromatography and molecular docking studies. Journal of Molecular Recognition, 2016, 29, 406-414.	1.1	15
32	Ionic Transport through Uncharged Nanopores. Biophysical Journal, 2016, 110, 655a.	0.2	0
33	Nanovectorization of DNA Through Cells Using Protamine Complexation. Journal of Membrane Biology, 2016, 249, 493-501.	1.0	5
34	Synthesis, regioselectivity, and DFT analysis of new antioxidant pyrazolo[4,3-c]quinoline-3,4-diones. Monatshefte FÃ¼r Chemie, 2016, 147, 1069-1079.	0.9	14
35	Biomimetic solution against dewetting in a highly hydrophobic nanopore. Soft Matter, 2016, 12, 4903-4911.	1.2	6
36	Encapsulation capacity and natural payload delivery of an anticancer drug from boron nitride nanotube. Physical Chemistry Chemical Physics, 2016, 18, 24994-25001.	1.3	49

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37	Electronic and optical properties of CeO₂ from first principles calculations. Analytical Methods, 2016, 8, 5045-5052.	1.3	29
38	Theoretical use of boron nitride nanotubes as a perfect container for anticancer molecules. Analytical Methods, 2016, 8, 1367-1372.	1.3	22
39	Towards New Insights in the Sterol/Amphotericin Nanochannels Formation: A Molecular Dynamic Simulation Study. Journal of Membrane Biology, 2016, 249, 261-270.	1.0	6
40	Carbon nanotube â€“ Protamine hybrid: Evaluation of DNA cell penetration. Carbon, 2016, 96, 742-752.	5.4	14
41	Selectivity against proton in cation permeable hybrid solid state membrane. Computational Materials Science, 2016, 111, 380-386.	1.4	4
42	Ionic transport through sub-10â€‰nm diameter hydrophobic high-aspect ratio nanopores: experiment, theory and simulation. Scientific Reports, 2015, 5, 10135.	1.6	72
43	Nanovector formation by functionalization of TRAIL ligand on single-walled carbon nanotube: Experimental and theoretical evidences. Chemical Physics Letters, 2015, 633, 273-281.	1.2	6
44	Nanovectorization of TRAIL with Single Wall Carbon Nanotubes Enhances Tumor Cell Killing. Nano Letters, 2015, 15, 891-895.	4.5	66
45	Theoretical study of the interaction between carbon nanotubes and carboplatin anticancer molecules. Analytical Methods, 2015, 7, 10145-10150.	1.3	21
46	Theoretical demonstration of the potentiality of boron nitride nanotubes to encapsulate anticancer molecule. Physical Chemistry Chemical Physics, 2015, 17, 30057-30064.	1.3	25
47	Encapsulation into Carbon Nanotubes and Release of Anticancer Cisplatin Drug Molecule. Journal of Physical Chemistry B, 2015, 119, 604-611.	1.2	74
48	Ionic selectivity of nystatin A1 confined in nanoporous trackâ€etched polymer membrane. IET Nanobiotechnology, 2014, 8, 138-142.	1.9	3
49	Quantum study of boron nitride nanotubes functionalized with anticancer molecules. Physical Chemistry Chemical Physics, 2014, 16, 18425-18432.	1.3	54
50	Supramolecular self-assembly of brominated molecules on a silicon surface. Chemical Communications, 2014, 50, 5714.	2.2	22
51	Experimental and simulation studies of unusual current blockade induced by translocation of small oxidized PEG through a single nanopore. Physical Chemistry Chemical Physics, 2014, 16, 17883.	1.3	11
52	Enhanced Ionic Transport Mechanism by Gramicidin A Confined Inside Nanopores Tuned by Atomic Layer Deposition. Journal of Physical Chemistry C, 2013, 117, 15306-15315.	1.5	39
53	Insertion kinetics of small nucleotides through single walled carbon nanotube. Journal of Biotechnology, 2013, 164, 13-18.	1.9	4
54	Efficiency of the monofunctionalized C60fullerenes as membrane targeting agents studied by all-atom molecular dynamics simulations. Molecular Membrane Biology, 2013, 30, 338-345.	2.0	5

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55	Enhanced potassium selectivity in a bioinspired solid nanopore. Physical Chemistry Chemical Physics, 2013, 15, 19601.	1.3	5
56	Structure and ionic selectivity of a hybrid polyene/artificial polymer solid state membrane. Soft Matter, 2013, 9, 684-691.	1.2	13
57	Theoretical study of amino derivatives and anticancer platinum drug grafted on various carbon nanostructures. Journal of Chemical Physics, 2013, 139, 174704.	1.2	12
58	Controlling potassium selectivity and proton blocking in a hybrid biological/solid-state polymer nanoporous membrane. Nanoscale, 2013, 5, 3961.	2.8	24
59	How long a functionalized carbon nanotube can passively penetrate a lipid membrane. Carbon, 2012, 50, 5301-5308.	5.4	26
60	Stability of the gramicidin-A channel structure in view of nanofiltration: a computational and experimental study. Soft Matter, 2011, 7, 10651.	1.2	6
61	New Bioinspired Membrane Made of a Biological Ion Channel Confined into the Cylindrical Nanopore of a Solid-State Polymer.. Nano Letters, 2011, 11, 712-716.	4.5	51
62	Formation of one-dimensional ordered alloy at step edges: An atomistic study of the (2Ã—1) Ni/Pt alloy on the Pt(997) surface. Surface Science, 2011, 605, 917-922.	0.8	17
63	Control of carbon nanotube handedness using a supramolecular chiral surface. Journal of Chemical Physics, 2011, 135, 154703.	1.2	3
64	Scaling of submonolayer island sizes in Ag growth on stepped Pt surfaces. Surface Science, 2010, 604, 1576-1583.	0.8	9
65	Modelling the Cu mono-atomic wire formation on Pt vicinal surfaces using kinetic Monte Carlo simulations. Modelling and Simulation in Materials Science and Engineering, 2010, 18, 085009.	0.8	7
66	Chiral interaction in double-wall carbon nanotubes: Simple rules deduced from a large sampling of tubes. Journal of Chemical Physics, 2010, 132, 124704.	1.2	3
67	A comparative study of single- and multiwalled carbon nanotube sensitivity to ammonia. Journal of Applied Physics, 2009, 105, .	1.1	11
68	Enantioselectivity of amino acids using chiral sensors based on nanotubes. Journal of Chemical Physics, 2009, 130, 114709.	1.2	10
69	Theoretical comparison between the response of single- and multiwalled carbon nanotubes based sensor as a function of the gas pressure. Sensors and Actuators A: Physical, 2009, 153, 37-41.	2.0	6
70	Growth of perfect and smooth Ag and Co monatomic wires on Pt vicinal surfaces: A kinetic Monte Carlo study. Surface Science, 2009, 603, 22-26.	0.8	13
71	Temperature effects on the growth of the Co adsorbates on Pt vicinal surface. Physics Procedia, 2009, 2, 865-872.	1.2	0
72	Theoretical study of the Ni growth on Pt stepped surfaces. Surface Science, 2009, 603, 2879-2887.	0.8	7

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73	Adsorption of Pt on Ni(111) surface: introduction of an effective pair interaction model. Physics Procedia, 2009, 2, 853-858.	1.2	0
74	Detection of amino acids encapsulation and adsorption with dielectric carbon nanotube. Journal of Biotechnology, 2009, 144, 96-101.	1.9	15
75	Multiwalled carbon nanotubes for dielectric sensing of biological systems: An effective treatment of polarization. Surface Science, 2008, 602, 235-240.	0.8	4
76	Conditions for organized nanoring growth using kinetic Monte Carlo simulations. Physical Review B, 2008, 77, .	1.1	3
77	Model for thermal desorption of hydrogen atoms from a graphite surface based on kinetic Monte Carlo simulations. Physical Review B, 2008, 77, .	1.1	22
78	Characterization of single wall carbon nanotubes by means of rare gas adsorption. Journal of Chemical Physics, 2007, 126, 054709.	1.2	13
79	First stages of epitaxial growth in the presence of an extended defect: Kinetic Monte Carlo simulations versus rate equation study on a vicinal surface. Physical Review B, 2007, 76, .	1.1	3
80	Chiral response of single walled carbon nanotube based sensors to adsorption of amino acids: A theoretical model. Journal of Chemical Physics, 2007, 127, 194702.	1.2	24
81	A Stable Roomâ€Temperature Molecular Assembly of Zwitterionic Organic Dipoles Guided by a Si(111)â€7Ã—7 Template Effect. Angewandte Chemie - International Edition, 2007, 46, 9287-9290.	7.2	32
82	Towards selective detection of chiral molecules using SWNT sensors. Surface Science, 2007, 601, 3818-3822.	0.8	17
83	Selective detection of chiral molecules by chiral single walled nanotubes. Chemical Physics Letters, 2007, 443, 113-117.	1.2	17
84	Determination of the single wall carbon nanotube opening ratio by means of rare gas adsorption. Chemical Physics Letters, 2006, 423, 183-186.	1.2	8
85	Direct growth of the multi-walled carbon nanotubes as a tool to detect ammonia at room temperature. Chemical Physics Letters, 2006, 433, 175-181.	1.2	55
86	Long nanotube dielectric properties used as sensors of large molecules: A semicontinuum approach. Journal of Chemical Physics, 2006, 125, 164708.	1.2	4
87	Zip gating of the KcsA channel studied by targeted molecular dynamics. Chemical Physics Letters, 2005, 407, 199-204.	1.2	4
88	Targeted molecular dynamics of an open-state KcsA channel. Journal of Chemical Physics, 2005, 122, 134707.	1.2	34
89	Alignment of single-wall carbon nanotubes by inclusion of dipolar wires. Physical Review B, 2005, 72, .	1.1	4
90	Gas-induced variation in the dielectric properties of carbon nanotube bundles for selective sensing. Journal of Applied Physics, 2005, 97, 114316.	1.1	38

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91	Influence of molecular adsorption on the dielectric properties of a single wall nanotube: A model sensor. Journal of Chemical Physics, 2004, 121, 9655-9665.	1.2	42
92	Grating formation in step flow heterogeneous growth and wavelength selection induced by confinement. Surface Science, 2004, 553, L68-L74.	0.8	7
93	Molecular selectivity due to adsorption properties in nanotubes. Physical Review B, 2004, 69, .	1.1	80
94	Theoretical study of conductance in stretched monatomic nanowires. Surface Science, 2003, 547, 249-256.	0.8	10
95	Improvement of nanowire distributions with a STM tip: a kinetic Monte Carlo approach. Surface Science, 2003, 532-535, 531-535.	0.8	0
96	Phonons softening in tip-stretched monatomic nanowires. Surface Science, 2003, 532-535, 544-548.	0.8	15
97	Can Kinetic Monte Carlo Simulation Help Experimentalists to Build Self-Organized Nanowires?. Physica Scripta, 2003, 68, C104-C107.	1.2	1
98	Complex band structures and decay length in polyethylene chains. Journal of Physics Condensed Matter, 2003, 15, 3731-3740.	0.7	38
99	Selective adsorption and structure formation ofN2on the nanostructured Cu-CuO stripe phase. Physical Review B, 2002, 66, .	1.1	15
100	Ordering of nitrogen molecules on the nanostructured Cu(110)/Cu(110)â€“(2Ã—1)O stripe phase. Surface Science, 2001, 482-485, 1379-1384.	0.8	2
101	Growth of composition-modulated Ag/Co wires on Pt(997). Physical Review B, 2001, 64, .	1.1	31
102	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.	1.1	33
103	Influence of step geometry and orientation on the growth of adsorbates. Surface Science, 2000, 454-456, 106-111.	0.8	2
104	Effect of the diffusion anisotropy on the nucleation and growth of xenon on Cu(110). Surface Science, 2000, 446, L113-L119.	0.8	14
105	INFLUENCE OF STEPS ON ATOMIC ADSORPTION AND SEQUENTIAL GROWTH ABOVE VICINAL SURFACES. Surface Review and Letters, 1999, 06, 669-681.	0.5	6
106	The primary structure of rabbit liver tRNAPhe and its comparison with known tRNAPhe sequences. FEBS Letters, 1973, 31, 345-347.	1.3	64