Solange B. Fagan

List of Publications by Year
in descending order

85 papers	3,066 citations	218381 26 h-index	161609 54 g-index
85 all docs	85 docs citations	85 times ranked	3712 citing authors

#	Article	IF	Citations
1	Methylphenidate adsorption onto graphene derivatives: theory and experiment. New Journal of Chemistry, 2022, 46, 4283-4291.	1.4	22
2	Influence of magnetite incorporation into chitosan on the adsorption of the methotrexate and in vitro cytotoxicity. Environmental Science and Pollution Research, 2022, 29, 70413-70434.	2.7	24
3	Adsorption of 17 Î²- estradiol in graphene oxide through the competing methanol co-solvent: Experimental and computational analysis. Journal of Molecular Liquids, 2021, 321, 114738.	2.3	24
4	Analysis of global and <scp>Latinâ€American</scp> trends in nanotoxicology with a focus on carbon nanomaterials: a scientometric approach. Journal of Chemical Technology and Biotechnology, 2021, 96, 2141-2151.	1.6	1
5	Theoretical study of small aromatic molecules adsorbed in pristine and functionalised graphene. Journal of Molecular Modeling, 2021, 27, 193.	0.8	8
6	A novel and green extraction strategy for sensitive determination of phthalates in aqueous samples: Analytical and computational studies. Microchemical Journal, 2021, 166, 106227.	2.3	2
7	Ab initio simulations of black and blue phosphorene functionalised with chemical groups for biomolecule anchoring. Journal of Molecular Modeling, 2021, 27, 349.	0.8	1
8	Computational Modeling of Environmental Co-exposure on Oil-Derived Hydrocarbon Overload by Using Substrate-Specific Transport Protein (TodX) with Graphene Nanostructures. Current Topics in Medicinal Chemistry, 2020, 20, 2308-2325.	1.0	3
9	Nanofilter based on functionalized carbon nanostructures for the adsorption of pentachlorophenol molecules. Computational and Theoretical Chemistry, 2019, 1165, 112561.	1.1	10
10	Density functional theory study of Ï€-aromatic interaction of benzene, phenol, catechol, dopamine isolated dimers and adsorbed on graphene surface. Journal of Molecular Modeling, 2019, 25, 302.	0.8	43
11	Interactions of graphene derivatives with glutamate-neurotransmitter: A parallel first principles - Docking investigation. Journal of Molecular Graphics and Modelling, 2019, 88, 121-127.	1.3	16
12	Computational MitoTarget Scanning Based on Topological Vacancies of Single-Walled Carbon Nanotubes with the Human Mitochondrial Voltage-Dependent Anion Channel (hVDAC1). Chemical Research in Toxicology, 2019, 32, 566-577.	1.7	4
13	History and National Initiatives of Carbon Nanotube and Graphene Research in Brazil. Brazilian Journal of Physics, 2019, 49, 288-300.	0.7	7
14	Modeling drug-drug interactions of AZD1208 with Vincristine and Daunorubicin on ligand-extrusion binding TMD-domains of multidrug resistance P-glycoprotein (ABCB1). Toxicology, 2019, 411, 81-92.	2.0	7
15	Ensino de NanociÃªncia e Nanotecnologia: perspectivas manifestadas por professores da educaÃ§Ã£o bÃ¡sica e superior. CiÃªncia & EducaÃ§Ã£o, 2019, 25, 665-683.	0.4	0
16	Carbon nanotubes functionalized with titanium complexes for hexavalent chromium adsorption: An ab initio approach. Computational and Theoretical Chemistry, 2017, 1113, 110-119.	1.1	6
17	The influence of the concentration and adsorption sites of different chemical groups on graphene through first principles simulations. Physical Chemistry Chemical Physics, 2017, 19, 27374-27383.	1.3	13
18	Adsorption of anti-inflammatory nimesulide by graphene materials: a combined theoretical and experimental study. Physical Chemistry Chemical Physics, 2017, 19, 22099-22110.	1.3	34

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19	A first-principles study of the interaction of doxorubicin with graphene. Computational and Theoretical Chemistry, 2017, 1115, 270-275.	1.1	24
20	Interaction of singleâ€walled carbon nanotubes and saxitoxin: Ab initio simulations and biological responses in hippocampal cell line HTâ€22. Environmental Toxicology and Chemistry, 2017, 36, 1728-1737.	2.2	5
21	Adsorption of Alizarin Red S Dye by Carbon Nanotubes: An Experimental and Theoretical Investigation. Journal of Physical Chemistry C, 2016, 120, 18296-18306.	1.5	103
22	Adsorption of sodium diclofenac on graphene: a combined experimental and theoretical study. Physical Chemistry Chemical Physics, 2016, 18, 1526-1536.	1.3	158
23	Adsorption of acridine orange and methylene blue synthetic dyes and anthracene on single wall carbon nanotubes: A first principle approach. Computational and Theoretical Chemistry, 2016, 1076, 42-50.	1.1	47
24	Interaction of <I>Î±</I>-Tocopherol with <I>Î±</I>- and <I>Î²</I>-Cyclodextrins: A First-Principles Investigation. Journal of Nanopharmaceutics and Drug Delivery, 2016, 3, 70-76.	0.3	5
25	Carboxylated Capped Carbon Nanotubes Interacting with Nimesulide Molecules: Applied Electric Fields Effects. Journal of Nanomaterials, 2015, 2015, 1-6.	1.5	0
26	Carbon Nanoadsorbents. Carbon Nanostructures, 2015, , 11-32.	0.1	15
27	Molecules with Biological Interest Adsorbed on Carbon Nanostructures. Carbon Nanostructures, 2015, , 107-122.	0.1	0
28	Adsorption of a textile dye from aqueous solutions by carbon nanotubes. Materials Research, 2014, 17, 153-160.	0.6	41
29	Pristine and functionalized capped carbon nanotubes under electric fields. Physica Status Solidi (B): Basic Research, 2014, 251, 649-654.	0.7	11
30	Influence of concentration and position of carboxyl groups on the electronic properties of single-walled carbon nanotubes. Physical Chemistry Chemical Physics, 2014, 16, 21602-21608.	1.3	13
31	Functionalization of carbon nanotube by carboxyl group under radial deformation. Chemical Physics, 2014, 428, 117-120.	0.9	22
32	Interactions of iron-oxide filled carbon nanotubes with gas molecules. Physical Chemistry Chemical Physics, 2013, 15, 14340.	1.3	2
33	First Principles Simulations of Zidovudine (AZT) Molecules Interacting with Carbon Nanostructures. Journal of Computational and Theoretical Nanoscience, 2013, 10, 313-317.	0.4	2
34	Carbon Nanostructures Interacting with Vitamins A, B3 and <I>C: Ab</I> Initio Simulations. Journal of Biomedical Nanotechnology, 2012, 8, 345-349.	0.5	8
35	Natural Lipid Nanoparticles Containing Nimesulide: Synthesis, Characterization and <I>In Vivo</I> Antiedematogenic and Antinociceptive Activities. Journal of Biomedical Nanotechnology, 2012, 8, 309-315.	0.5	23
36	Adsorption of Reactive Blue 4 dye from water solutions by carbon nanotubes: experiment and theory. Physical Chemistry Chemical Physics, 2012, 14, 11139.	1.3	155

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37	Metal-doped carbon nanotubes interacting with vitamin C. Physical Chemistry Chemical Physics, 2012, 14, 16737.	1.3	5
38	Selenium Nanostructures Adsorbed on Carbon Nanotubes: A DFT Investigation. Journal of Computational and Theoretical Nanoscience, 2011, 8, 1710-1715.	0.4	0
39	Adsorption of Reactive Red M-2BE dye from water solutions by multi-walled carbon nanotubes and activated carbon. Journal of Hazardous Materials, 2011, 192, 1122-1131.	6.5	309
40	Electronic transport properties of ascorbic acid and nicotinamide adsorbed on single-walled carbon nanotubes. Chemical Physics Letters, 2011, 506, 233-238.	1.2	13
41	Magnetization profile for impurities in graphene nanoribbons. Physical Review B, 2011, 84, .	1.1	20
42	Nicotine adsorption on single wall carbon nanotubes. Journal of Hazardous Materials, 2010, 184, 678-683.	6.5	19
43	Chlorophyll a and pheophytin a as gas sensors of CO2 and O2 molecules. Chemical Physics Letters, 2010, 496, 310-315.	1.2	5
44	First Principles Study of Transverse Electric Fields on Carbon Nanotubes. , 2010, , .		2
45	Benzonitrile Adsorption on Fe-Doped Carbon Nanostructures. Journal of Physical Chemistry C, 2010, 114, 10790-10795.	1.5	18
46	Functionalization of single-wall carbon nanotubes through chloroform adsorption: theory and experiment. Physical Chemistry Chemical Physics, 2010, 12, 1518.	1.3	27
47	Model of impurity segregation in graphene nanoribbons. Physical Review B, 2009, 80, .	1.1	14
48	Resonance Raman spectroscopy in Si and C ion-implanted double-wall carbon nanotubes. Physical Review B, 2009, 80, .	1.1	19
49	Non-covalent interaction of benzonitrile with single-walled carbon nanotubes. Journal of Nanoparticle Research, 2009, 11, 2163-2170.	0.8	5
50	Anchoring Silanols Radicals on Carbon Nanotubes. Journal of Computational and Theoretical Nanoscience, 2009, 6, 548-551.	0.4	0
51	Carboxylated Carbon Nanotubes under External Electrical Field: An Ab Initio Investigation. Journal of Physical Chemistry C, 2009, 113, 8959-8963.	1.5	13
52	Chemical doping-induced gap opening and spin polarization in graphene. Physical Review B, 2008, 77, .	1.1	128
53	Switching on magnetism in Ni-doped graphene: Density functional calculations. Physical Review B, 2008, 78, .	1.1	83
54	Electronic and Magnetic Properties of Ti and Fe on Graphene. Journal of Physical Chemistry C, 2008, 112, 9163-9167.	1.5	91

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55	Ab Initio Study of SO₂ Molecules Interacting with Pristine and Transition Metal Covered Fullerenes as a Possible Route for Nanofilters. Journal of Physical Chemistry C, 2008, 112, 6677-6680.	1.5	5
56	First Principles Calculations of Alanine Radicals Adsorbed on Pristine and Functionalized Carbon Nanotubes. Journal of Physical Chemistry C, 2008, 112, 14812-14815.	1.5	11
57	FuncionalizaÃ§Ã£o de nanotubos de Carbono. Quimica Nova, 2007, 30, 1695-1703.	0.3	28
58	Encapsulation of Metallocenes in Single-Wall Carbon Nanotubes: an Ab Initio Study. AIP Conference Proceedings, 2007, , .	0.3	1
59	First principles study of titanium-coated carbon nanotubes as sensors for carbon monoxide molecules. Surface Science, 2007, 601, 4102-4104.	0.8	23
60	Ab initio study of 2,3,7,8-tetrachlorinated dibenzo-p-dioxin adsorption on single wall carbon nanotubes. Chemical Physics Letters, 2007, 437, 79-82.	1.2	41
61	Ab initio study of pristine and Si-doped capped carbon nanotubes interacting with nimesulide molecules. Chemical Physics Letters, 2007, 439, 348-353.	1.2	39
62	Ab initio study of double-wall carbon nanotubes under uniaxial pressure. Physica Status Solidi (B): Basic Research, 2007, 244, 142-146.	0.7	2
63	Interaction of a methanol molecule with C60 under pressure. Physica Status Solidi (B): Basic Research, 2007, 244, 151-155.	0.7	1
64	First principles study of 1,2-dichlorobenzene adsorption on metallic carbon nanotubes. International Journal of Quantum Chemistry, 2006, 106, 2558-2563.	1.0	23
65	Ab initio study of covalently functionalized carbon nanotubes. Chemical Physics Letters, 2006, 430, 71-74.	1.2	86
66	Silicon adsorption in defective carbon nanotubes: a first principles study. Nanotechnology, 2006, 17, 4088-4091.	1.3	4
67	Titanium monomers and wires adsorbed on carbon nanotubes: a first principles study. Nanotechnology, 2006, 17, 1154-1159.	1.3	22
68	Lithium intercalation into single-wall carbon nanotube bundles. Microelectronics Journal, 2005, 36, 499-501.	1.1	17
69	Electronic properties of Ag- and CrO3-filled single-wall carbon nanotubes. Chemical Physics Letters, 2005, 406, 54-59.	1.2	63
70	Electronic properties ofFeCl3-adsorbed single-wall carbon nanotubes. Physical Review B, 2005, 72, .	1.1	11
71	Ab initiocalculations ofCaCu3Ti4O12under high pressure: Structural and electronic properties. Physical Review B, 2005, 72, .	1.1	19
72	Anab initiostudy of manganese atoms and wires interacting with carbon nanotubes. Journal of Physics Condensed Matter, 2004, 16, 3647-3661.	0.7	16

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73	1,2-Dichlorobenzene Interacting with Carbon Nanotubes. Nano Letters, 2004, 4, 1285-1288.	4.5	153
74	Ab Initio Study of Deformed Carbon Nanotube Sensors for Carbon Monoxide Molecules. Nano Letters, 2004, 4, 65-67.	4.5	111
75	Substitutional Si Doping in Deformed Carbon Nanotubes. Nano Letters, 2004, 4, 975-977.	4.5	48
76	Raman scattering and x-ray diffraction studies of polycrystallineCaCu3Ti4O12under high-pressure. Physical Review B, 2004, 70, .	1.1	56
77	Ab initio Study of Radial Deformation Plus Vacancy on Carbon Nanotubes:Â Energetics and Electronic Properties. Nano Letters, 2003, 3, 289-291.	4.5	40
78	Energetics and structural properties of adsorbed atoms and molecules on silicon-doped carbon nanotubes. Materials Characterization, 2003, 50, 183-187.	1.9	24
79	Fe and Mn atoms interacting with carbon nanotubes. Physica B: Condensed Matter, 2003, 340-342, 982-985.	1.3	20
80	Electronic and magnetic properties of iron chains on carbon nanotubes. Microelectronics Journal, 2003, 34, 481-484.	1.1	34
81	Ab initiostudy of an iron atom interacting with single-wall carbon nanotubes. Physical Review B, 2003, 67, .	1.1	101
82	Ab initio study of an organic molecule interacting with a silicon-doped carbon nanotube. Diamond and Related Materials, 2003, 12, 861-863.	1.8	21
83	Functionalization of carbon nanotubes through the chemical binding of atoms and molecules. Physical Review B, 2003, 67, .	1.1	67
84	Electronic and structural properties of silicon-doped carbon nanotubes. Physical Review B, 2001, 64, .	1.1	109
85	Ab initiocalculations for a hypothetical material: Silicon nanotubes. Physical Review B, 2000, 61, 9994-9996.	1.1	240