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	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
2	Ab initiocalculations for a hypothetical material: Silicon nanotubes. Physical Review B, 2000, 61, 9994-9996.	1.1	240
3	Adsorption of sodium diclofenac on graphene: a combined experimental and theoretical study. Physical Chemistry Chemical Physics, 2016, 18, 1526-1536.	1.3	158
4	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
5	1,2-Dichlorobenzene Interacting with Carbon Nanotubes. Nano Letters, 2004, 4, 1285-1288.	4.5	153
6	Chemical doping-induced gap opening and spin polarization in graphene. Physical Review B, 2008, 77, .	1.1	128
7	Ab Initio Study of Deformed Carbon Nanotube Sensors for Carbon Monoxide Molecules. Nano Letters, 2004, 4, 65-67.	4.5	111
8	Electronic and structural properties of silicon-doped carbon nanotubes. Physical Review B, 2001, 64, .	1.1	109
9	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
10	Ab initiostudy of an iron atom interacting with single-wall carbon nanotubes. Physical Review B, 2003, 67, .	1.1	101
11	Electronic and Magnetic Properties of Ti and Fe on Graphene. Journal of Physical Chemistry C, 2008, 112, 9163-9167.	1.5	91
12	Ab initio study of covalently functionalized carbon nanotubes. Chemical Physics Letters, 2006, 430, 71-74.	1.2	86
13	Switching on magnetism in Ni-doped graphene: Density functional calculations. Physical Review B, 2008, 78, .	1.1	83
14	Functionalization of carbon nanotubes through the chemical binding of atoms and molecules. Physical Review B, 2003, 67, .	1.1	67
15	Electronic properties of Ag- and CrO3-filled single-wall carbon nanotubes. Chemical Physics Letters, 2005, 406, 54-59.	1.2	63
16	Raman scattering and x-ray diffraction studies of polycrystallineCaCu3Ti4O12under high-pressure. Physical Review B, 2004, 70, .	1.1	56
17	Substitutional Si Doping in Deformed Carbon Nanotubes. Nano Letters, 2004, 4, 975-977.	4.5	48
18	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

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19	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
20	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
21	Adsorption of a textile dye from aqueous solutions by carbon nanotubes. Materials Research, 2014, 17, 153-160.	0.6	41
22	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
23	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
24	Electronic and magnetic properties of iron chains on carbon nanotubes. Microelectronics Journal, 2003, 34, 481-484.	1.1	34
25	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
26	FuncionalizaÃ§Ã£o de nanotubos de Carbono. Quimica Nova, 2007, 30, 1695-1703.	0.3	28
27	Functionalization of single-wall carbon nanotubes through chloroform adsorption: theory and experiment. Physical Chemistry Chemical Physics, 2010, 12, 1518.	1.3	27
28	Energetics and structural properties of adsorbed atoms and molecules on silicon-doped carbon nanotubes. Materials Characterization, 2003, 50, 183-187.	1.9	24
29	A first-principles study of the interaction of doxorubicin with graphene. Computational and Theoretical Chemistry, 2017, 1115, 270-275.	1.1	24
30	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
31	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
32	First principles study of 1,2-dichlorobenzene adsorption on metallic carbon nanotubes. International Journal of Quantum Chemistry, 2006, 106, 2558-2563.	1.0	23
33	First principles study of titanium-coated carbon nanotubes as sensors for carbon monoxide molecules. Surface Science, 2007, 601, 4102-4104.	0.8	23
34	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
35	Titanium monomers and wires adsorbed on carbon nanotubes: a first principles study. Nanotechnology, 2006, 17, 1154-1159.	1.3	22
36	Functionalization of carbon nanotube by carboxyl group under radial deformation. Chemical Physics, 2014, 428, 117-120.	0.9	22

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37	Methylphenidate adsorption onto graphene derivatives: theory and experiment. New Journal of Chemistry, 2022, 46, 4283-4291.	1.4	22
38	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
39	Fe and Mn atoms interacting with carbon nanotubes. Physica B: Condensed Matter, 2003, 340-342, 982-985.	1.3	20
40	Magnetization profile for impurities in graphene nanoribbons. Physical Review B, 2011, 84, .	1.1	20
41	Ab initiocalculations ofCaCu3Ti4O12under high pressure: Structural and electronic properties. Physical Review B, 2005, 72, .	1.1	19
42	Resonance Raman spectroscopy in Si and C ion-implanted double-wall carbon nanotubes. Physical Review B, 2009, 80, .	1.1	19
43	Nicotine adsorption on single wall carbon nanotubes. Journal of Hazardous Materials, 2010, 184, 678-683.	6.5	19
44	Benzonitrile Adsorption on Fe-Doped Carbon Nanostructures. Journal of Physical Chemistry C, 2010, 114, 10790-10795.	1.5	18
45	Lithium intercalation into single-wall carbon nanotube bundles. Microelectronics Journal, 2005, 36, 499-501.	1.1	17
46	Anab initiostudy of manganese atoms and wires interacting with carbon nanotubes. Journal of Physics Condensed Matter, 2004, 16, 3647-3661.	0.7	16
47	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
48	Carbon Nanoadsorbents. Carbon Nanostructures, 2015, , 11-32.	0.1	15
49	Model of impurity segregation in graphene nanoribbons. Physical Review B, 2009, 80, .	1.1	14
50	Carboxylated Carbon Nanotubes under External Electrical Field: An Ab Initio Investigation. Journal of Physical Chemistry C, 2009, 113, 8959-8963.	1.5	13
51	Electronic transport properties of ascorbic acid and nicotinamide adsorbed on single-walled carbon nanotubes. Chemical Physics Letters, 2011, 506, 233-238.	1.2	13
52	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
53	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
54	Electronic properties ofFeCl3-adsorbed single-wall carbon nanotubes. Physical Review B, 2005, 72, .	1.1	11

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55	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
56	Pristine and functionalized capped carbon nanotubes under electric fields. Physica Status Solidi (B): Basic Research, 2014, 251, 649-654.	0.7	11
57	Nanofilter based on functionalized carbon nanostructures for the adsorption of pentachlorophenol molecules. Computational and Theoretical Chemistry, 2019, 1165, 112561.	1.1	10
58	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
59	Theoretical study of small aromatic molecules adsorbed in pristine and functionalised graphene. Journal of Molecular Modeling, 2021, 27, 193.	0.8	8
60	History and National Initiatives of Carbon Nanotube and Graphene Research in Brazil. Brazilian Journal of Physics, 2019, 49, 288-300.	0.7	7
61	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
62	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
63	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
64	Non-covalent interaction of benzonitrile with single-walled carbon nanotubes. Journal of Nanoparticle Research, 2009, 11, 2163-2170.	0.8	5
65	Chlorophyll a and pheophytin a as gas sensors of CO2 and O2 molecules. Chemical Physics Letters, 2010, 496, 310-315.	1.2	5
66	Metal-doped carbon nanotubes interacting with vitamin C. Physical Chemistry Chemical Physics, 2012, 14, 16737.	1.3	5
67	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
68	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
69	Silicon adsorption in defective carbon nanotubes: a first principles study. Nanotechnology, 2006, 17, 4088-4091.	1.3	4
70	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
71	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
72	Ab initio study of double-wall carbon nanotubes under uniaxial pressure. Physica Status Solidi (B): Basic Research, 2007, 244, 142-146.	0.7	2

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73	First Principles Study of Transverse Electric Fields on Carbon Nanotubes. , 2010, , .		2
74	Interactions of iron-oxide filled carbon nanotubes with gas molecules. Physical Chemistry Chemical Physics, 2013, 15, 14340.	1.3	2
75	First Principles Simulations of Zidovudine (AZT) Molecules Interacting with Carbon Nanostructures. Journal of Computational and Theoretical Nanoscience, 2013, 10, 313-317.	0.4	2
76	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
77	Encapsulation of Metallocenes in Single-Wall Carbon Nanotubes: an Ab Initio Study. AIP Conference Proceedings, 2007, , .	0.3	1
78	Interaction of a methanol molecule with C60 under pressure. Physica Status Solidi (B): Basic Research, 2007, 244, 151-155.	0.7	1
79	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
80	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
81	Anchoring Silanols Radicals on Carbon Nanotubes. Journal of Computational and Theoretical Nanoscience, 2009, 6, 548-551.	0.4	0
82	Selenium Nanostructures Adsorbed on Carbon Nanotubes: A DFT Investigation. Journal of Computational and Theoretical Nanoscience, 2011, 8, 1710-1715.	0.4	0
83	Carboxylated Capped Carbon Nanotubes Interacting with Nimesulide Molecules: Applied Electric Fields Effects. Journal of Nanomaterials, 2015, 2015, 1-6.	1.5	0
84	Molecules with Biological Interest Adsorbed on Carbon Nanostructures. Carbon Nanostructures, 2015, , 107-122.	0.1	0
85	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