Caetano R Miranda

List of Publications by Year
in descending order

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86 papers	2,196 citations	279798 23 h-index	254184 43 g-index
87 all docs	87 docs citations	87 times ranked	2920 citing authors

#	Article	IF	Citations
1	The role of topological defects on the mechanical properties of single-walled carbon nanotubes. Philosophical Magazine, 2022, 102, 210-227.	1.6	3
2	First-principles calculations of carboxylic acid adsorption on carbonate surfaces: Chain size and aqueous interface effects. Applied Surface Science, 2022, , 153216.	6.1	1
3	Effects of <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msup><mml:mrow><mml:mi>Ca</mml:mi></mml:mrow><mml:mrow><mml substitution on the properties of cementitious tobermorite. Physical Review Materials, 2022, 6, .	2.4	2
4	Experimental and computational investigation of Ti-Nb-Fe-Zr alloys with limited Fe contents for biomedical applications. Journal of Materials Science, 2021, 56, 11494-11510.	3.7	4
5	Electronic Structure of Water from Koopmans-Compliant Functionals. Journal of Chemical Theory and Computation, 2021, 17, 3923-3930.	5.3	6
6	Probing the dynamics of water over multiple pore scales in cement by atomistic simulations. Applied Surface Science, 2021, 565, 150426.	6.1	10
7	Mechanism for enhanced oil recovery from carbonate reservoirs by adding copper ions to seawater. Fuel, 2021, 305, 121605.	6.4	3
8	CO2 Adsorption Enhanced by Tuning the Layer Charge in a Clay Mineral. Langmuir, 2021, , .	3.5	11
9	CO₂ Capture by Nickel Hydroxide Interstratified in the Nanolayered Space of a Synthetic Clay Mineral. Journal of Physical Chemistry C, 2020, 124, 26222-26231.	3.1	12
10	Nanoalloys for Energy Applications. , 2020, , 347-380.		3
11	Discovery of Low-Modulus Ti-Nb-Zr Alloys Based on Machine Learning and First-Principles Calculations. ACS Applied Materials & Interfaces, 2020, 12, 56850-56861.	8.0	20
12	Brineâ€“Oil Interfacial Tension Modeling: Assessment of Machine Learning Techniques Combined with Molecular Dynamics. ACS Applied Materials & Interfaces, 2020, 12, 15837-15843.	8.0	19
13	Multiscale Molecular Modeling Applied to the Upstream Oil & Gas Industry Challenges. Polytechnica, 2020, 3, 54-65.	2.1	5
14	Selective dissociation of benzoic acid on carbonate surfaces: A density functional theory perspective. Applied Surface Science, 2020, 529, 147103.	6.1	5
15	Confinement and hydrophilicity effects on geologically relevant fluids in silica nanopores. Physical Review Fluids, 2020, 5, .	2.5	3
16	On the Mechanism of Carbon Dioxide Reduction on Sn-Based Electrodes: Insights into the Role of Oxide Surfaces. Catalysts, 2019, 9, 636.	3.5	21
17	From Atoms to Pre-salt Reservoirs: Multiscale Simulations of the Low-Salinity Enhanced Oil Recovery Mechanisms. Polytechnica, 2019, 2, 30-50.	2.1	3
18	Uncovering the Mechanisms of Low-Salinity Water Injection EOR Processes: A Molecular Simulation Viewpoint. , 2019, , .		2

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19	Multiscale Coupling between Molecular Simulations and Reservoir Simulator: Geochemical Reactions for Low Salinity Water Injection in Carbonates. , 2019, , .		0
20	Ab Initio Molecular Dynamics Study of Carbonation and Hydrolysis Reactions on Cleaved Quartz (001) Surface. Journal of Physical Chemistry C, 2019, 123, 4938-4948.	3.1	12
21	Ethanol chemisorption on coreâ€“shell Pt-nanoparticles: an ab initio study. European Physical Journal B, 2019, 92, 1.	1.5	6
22	Virtual Reality for Visualization of Enhanced Oil Recovery Processes at Nanoscale. , 2019, , .		0
23	The surface stability and morphology of tobermorite 11â€Ã... from first principles. Applied Surface Science, 2018, 444, 287-292.	6.1	15
24	Fresh Molecular Look at Calciteâ€“Brine Nanoconfined Interfaces. Journal of Physical Chemistry C, 2018, 122, 6117-6127.	3.1	25
25	Multilevel Molecular Modeling Approach for a Rational Design of Ionic Current Sensors for Nanofluidics. Journal of Chemical Theory and Computation, 2018, 14, 3113-3120.	5.3	6
26	The role of Cr on the electronic and optical properties of InCrN: A first principles study. Journal of Crystal Growth, 2018, 499, 13-17.	1.5	4
27	Evaluation of Cyclodextrins as Environmentally Friendly Wettability Modifiers for Enhanced Oil Recovery. Colloids and Interfaces, 2018, 2, 10.	2.1	5
28	Theory as a driving force to understand reactions on nanoparticles: general discussion. Faraday Discussions, 2018, 208, 147-185.	3.2	3
29	Application of new nanoparticle structures as catalysts: general discussion. Faraday Discussions, 2018, 208, 575-593.	3.2	1
30	Nanoscience Applied to Oil Recovery and Mitigation: A Multiscale Computational Approach. MRS Advances, 2017, 2, 477-482.	0.9	6
31	Theoretical Study of Hydrogen Adsorption on Au@Pd Icosahedral Nanoparticle. Journal of Physical Chemistry C, 2017, 121, 8613-8622.	3.1	14
32	Molecular Dynamics Simulations of Water Confined in Calcite Slit Pores: An NMR Spin Relaxation and Hydrogen Bond Analysis. Journal of Physical Chemistry C, 2017, 121, 6674-6684.	3.1	40
33	From Single Asphaltenes and Resins to Nanoaggregates: A Computational Study. Energy & Fuels, 2017, 31, 11743-11754.	5.1	22
34	Controlling Clay Swellingâ€“Shrinkage with Inorganic Nanoparticles: A Molecular Dynamics Study. Journal of Physical Chemistry C, 2017, 121, 20266-20271.	3.1	16
35	Molecular simulations of cement based materials: A comparison between first principles and classical force field calculations. Computational Materials Science, 2017, 138, 392-402.	3.0	36
36	Multiple pathways in pressure-induced phase transition of coesite. Proceedings of the National Academy of Sciences of the United States of America, 2017, 114, 12894-12899.	7.1	7

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37	Retention of contaminants Cd and Hg adsorbed and intercalated in aluminosilicate clays: A first principles study. Journal of Chemical Physics, 2017, 147, 174704.	3.0	5
38	Improved oil recovery in nanopores: NanoIOR. Scientific Reports, 2016, 6, 28128.	3.3	29
39	Adsorption of asphaltenes on the calcite (10.4) surface by first-principles calculations. RSC Advances, 2016, 6, 95328-95336.	3.6	31
40	Hosting of La3+ guest ions in type-I Ge clathrates: A first-principles characterization for thermoelectric applications. Computational Materials Science, 2016, 122, 46-56.	3.0	4
41	Noncontact AFM First-Principles Simulations of Functionalized Silicon Tips on the Montmorillonite (001) Surface. Journal of Physical Chemistry C, 2016, 120, 13503-13513.	3.1	7
42	Combining molecular dynamics and lattice Boltzmann simulations: a hierarchical computational protocol for microfluidics. Microfluidics and Nanofluidics, 2016, 20, 1.	2.2	8
43	Functionalized Silica Nanoparticles within Multicomponent Oil/Brine Interfaces: A Study in Molecular Dynamics. Journal of Physical Chemistry C, 2016, 120, 6787-6795.	3.1	20
44	First principles characterization of silicate sites in clay surfaces. Physical Chemistry Chemical Physics, 2015, 17, 4952-4960.	2.8	21
45	Potential applications of cyclodextrins in enhanced oil recovery. Colloids and Surfaces A: Physicochemical and Engineering Aspects, 2015, 469, 42-50.	4.7	18
46	First-Principles Investigation of Transition Metal Dichalcogenide Nanotubes for Li and Mg Ion Battery Applications. Journal of Physical Chemistry C, 2015, 119, 4302-4311.	3.1	47
47	Molecular dynamics studies of aqueous silica nanoparticle dispersions: salt effects on the double layer formation. Journal of Physics Condensed Matter, 2015, 27, 325101.	1.8	15
48	Atomistic pathways of the pressure-induced densification of quartz. Physical Review B, 2015, 92, .	3.2	6
49	The stability and interfacial properties of functionalized silica nanoparticles dispersed in brine studied by molecular dynamics. European Physical Journal B, 2015, 88, 1.	1.5	13
50	NMR characterization of hydrocarbon adsorption on calcite surfaces: A first principles study. Journal of Chemical Physics, 2014, 141, 204705.	3.0	14
51	Aggregation kinetics and shear rheology of aqueous silica suspensions. Applied Nanoscience (Switzerland), 2014, 4, 169-178.	3.1	43
52	Modeling Acid Oil Component Interactions with Carbonate Reservoirs: A First-Principles View on Low Salinity Recovery Mechanisms. Journal of Physical Chemistry C, 2014, 118, 19180-19187.	3.1	39
53	Atomic scale insights into ethanol oxidation on Pt, Pd and Au metallic nanofilms: A DFT with van der Waals interactions. Applied Surface Science, 2014, 288, 564-571.	6.1	39
54	Energetics of formation and hydration of functionalized silica nanoparticles: An atomistic computational study. Applied Surface Science, 2014, 292, 742-749.	6.1	20

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55	First-principles calculations of H, O and OH adsorption on metallic layered supported thin films. Journal of Physics Condensed Matter, 2013, 25, 175002.	1.8	6
56	Comparison of thermodynamic stabilities and mechanical properties of CO2, SiO2, and GeO2 polymorphs by first-principles calculations. Journal of Chemical Physics, 2012, 137, 034703.	3.0	2
57	Hydrocarbon Adsorption on Carbonate Mineral Surfaces: A First-Principles Study with van der Waals Interactions. Journal of Physical Chemistry C, 2012, 116, 24538-24548.	3.1	34
58	Interface tension of silica hydroxylated nanoparticle with brine: A combined experimental and molecular dynamics study. Journal of Chemical Physics, 2012, 136, 164702.	3.0	24
59	Molecular Dynamics Studies of Fluid/Oil Interfaces for Improved Oil Recovery Processes. Journal of Physical Chemistry B, 2012, 116, 14667-14676.	2.6	126
60	Stability and Mobility of Functionalized Silica Nanoparticles for Enhanced Oil Recovery Applications. , 2012, , .		92
61	Stability of aqueous silica nanoparticle dispersions. Journal of Nanoparticle Research, 2011, 13, 839-850.	1.9	254
62	Structural properties and phase transitions in a silica clathrate. Journal of Chemical Physics, 2011, 134, 074506.	3.0	5
63	Combined modeling and experimental studies of hydroxylated silica nanoparticles. Journal of Materials Science, 2010, 45, 5084-5088.	3.7	27
64	Self-Accumulation of Aromatics at the Oilâ^'Water Interface through Weak Hydrogen Bonding. Journal of the American Chemical Society, 2010, 132, 18281-18286.	13.7	180
65	Measurement of the SiCl₄ Diffusion Coefficient in a Room-Temperature Ionic Liquid by an Optical MoirÃ©-Pattern Technique. ECS Transactions, 2009, 16, 13-23.	0.5	1
66	Infrared absorption of MgO at high pressures and temperatures: A molecular dynamic study. Journal of Chemical Physics, 2009, 131, 014506.	3.0	15
67	<i>In Situ</i> Raman Spectroscopy Studies of the Electrolyte-Substrate Interface during Electrodeposition of Silicon in a Room-Temperature Ionic Liquid. ECS Transactions, 2009, 16, 1-6.	0.5	15
68	Effect of particle size and surface structure on adsorption of O and OH on platinum nanoparticles: A first-principles study. Physical Review B, 2008, 77, .	3.2	173
69	Temperature-induced densification of compressed SiO₂glass: A molecular dynamics study. High Pressure Research, 2008, 28, 35-44.	1.2	19
70	Tuning Oxygen Packing in Silica by Nonhydrostatic Pressure. Physical Review Letters, 2007, 99, 215504.	7.8	34
71	Mechanical strength and coordination defects in compressed silica glass: Molecular dynamics simulations. Physical Review B, 2007, 75, .	3.2	91
72	An Ab Initio Study of Lithium Diffusion in Titanium Disulfide Nanotubes. Chemistry of Materials, 2007, 19, 5302-5308.	6.7	46

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73	Ab initio investigation of ammonia-borane complexes for hydrogen storage. Journal of Chemical Physics, 2007, 126, 184703.	3.0	116
74	Thermodynamics of type-I and type-II Si clathrates at zero pressure: Monte Carlo simulations. Physical Review B, 2006, 74, .	3.2	11
75	Infrared and Raman spectra of silica polymorphs from anab initioparametrized polarizable force field. Journal of Chemical Physics, 2006, 125, 194524.	3.0	54
76	A computational study of elastic properties of disordered systems with voids. Journal of Non-Crystalline Solids, 2006, 352, 4283-4286.	3.1	10
77	Computational materials science meets geophysics: dislocations and slip planes of MgO. Computer Physics Communications, 2005, 169, 24-27.	7.5	30
78	Comment on â€œa/[110]Stacking Fault Model for Platelets in Diamondâ€• Physical Review Letters, 2005, 95, 139601; author reply 139602.	7.8	2
79	Transitions between disordered phases in supercooled liquid silicon. Journal of Chemical Physics, 2004, 120, 11672-11677.	3.0	40
80	Stacking-Fault Based Microscopic Model for Platelets in Diamond. Physical Review Letters, 2004, 93, 265502.	7.8	9
81	Vacancy-like defects in a-Si: a first principles study. Journal of Non-Crystalline Solids, 2004, 338-340, 400-402.	3.1	11
82	Temperature effects on dislocation core energies in silicon and germanium. Physical Review B, 2003, 67, .	3.2	18
83	Atomistic prediction of equilibrium vacancy concentrations inNi3Al. Physical Review B, 2002, 66, .	3.2	20
84	Thermodynamics of supercooled liquid silicon and its glass transition. Materials Research Society Symposia Proceedings, 2002, 754, 1.	0.1	0
85	Multiscale fluid dynamics in porous media: applications in enhanced oil recovery. Anais Do ... Congresso Ibero-Latino-Americano De MÃ©todos Computacionais Em Engenharia, 0, , .	0.0	1
86	Women in science: a brazilian experience through immersive narratives in 360Â° videos. International Journal of Science Education, Part B: Communication and Public Engagement, 0, , 1-19.	1.5	0