Gustavo T Troiano Feliciano

List of Publications by Year
in descending order

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30 papers	581 citations	840776 11 h-index	610901 24 g-index
30 all docs	30 docs citations	30 times ranked	792 citing authors

#	Article	IF	Citations
1	Molecular dynamics investigation of the structural and energetic properties of CeO₂â€“MO_x (M = Gd, La, Ce, Zr) nanoparticles. Materials Advances, 2021, 2, 7759-7772.	5.4	6
2	Thermodynamic and structural aspects of molecular recognition in mannose-binding protein complexes: a theoretical study over HRP-ArtinM association. Journal of Molecular Modeling, 2021, 27, 107.	1.8	1
3	Low-fouling properties in serum of carboxylic-oligo(ethylene glycol)-based interfaces. Colloids and Surfaces A: Physicochemical and Engineering Aspects, 2021, 618, 126426.	4.7	0
4	Steric and Electrostatic Effects on the Diffusion of CH4/CH3OH in Copper-Exchanged Zeolites: Insights from Enhanced Sampling Molecular Dynamics and Free Energy Calculations. Langmuir, 2021, 37, 8014-8023.	3.5	1
5	Atomic and Electronic Structure of Pilus from Geobacter sulfurreducens through QM/MM Calculations: Evidence for Hole Transfer in Aromatic Residues. Journal of Physical Chemistry B, 2021, 125, 8305-8312.	2.6	8
6	Optical and electronic properties of TiO2/GOQDs composites: A combined experimental and first-principles calculations study. Computational Materials Science, 2021, 195, 110503.	3.0	11
7	Genetic Algorithms Applied to Thermodynamic Rational Design of Mimetic Antibodies Based on the GB1 Domain of Streptococcal Protein G: An Atomistic Simulation Study. Journal of Physical Chemistry B, 2021, 125, 7985-7996.	2.6	0
8	The density-of-States and equilibrium charge dynamics of redox-active switches. Electrochimica Acta, 2021, 387, 138410.	5.2	8
9	Experimental and molecular dynamics study of graphene oxide quantum dots interaction with solvents and its aggregation mechanism. Journal of Molecular Liquids, 2021, 335, 116136.	4.9	5
10	Three-dimensional catalysis and the efficient bioelectrocatalysis beyond surface chemistry. Journal of Catalysis, 2021, 401, 200-205.	6.2	8
11	Ab Initio QM/MM Simulation of Ferrocene Homogeneous Electron-Transfer Reaction. Journal of Physical Chemistry A, 2021, 125, 25-33.	2.5	7
12	Multidimensional redox potential/pKa coupling in multicopper oxidases from molecular dynamics: implications for the proton transfer mechanism. Physical Chemistry Chemical Physics, 2021, , .	2.8	0
13	The role of water on the electronic transport in graphene nanogap devices designed for DNA sequencing. Carbon, 2020, 158, 314-319.	10.3	17
14	Two-Dimensional Nature and the Meaning of the Density of States in Redox Monolayers. Journal of Physical Chemistry C, 2020, 124, 14918-14927.	3.1	6
15	Exploring Coupled Redox and pH Processes with a Force-Field-Based Approach: Applications to Five Different Systems. Journal of the American Chemical Society, 2020, 142, 3823-3835.	13.7	15
16	Simulating DNA Chip Design Using All-Electronic Graphene-Based Substrates. Molecules, 2019, 24, 951.	3.8	6
17	Addressing the Environment Electrostatic Effect on Ballistic Electron Transport in Large Systems: A QM/MM-NEGF Approach. Journal of Physical Chemistry B, 2018, 122, 485-492.	2.6	21
18	Mapping the ionic fingerprints of molecular monolayers. Physical Chemistry Chemical Physics, 2017, 19, 15098-15109.	2.8	22

#	Article	IF	Citations
19	Caprylate Salts Based on Amines as Volatile Corrosion Inhibitors for Metallic Zinc: Theoretical and Experimental Studies. Frontiers in Chemistry, 2017, 5, 32.	3.6	6
20	Development of a biomimetic sensor for selective identification of cyanide. Analytical Methods, 2016, 8, 6353-6360.	2.7	11
21	Thermally activated charge transport in microbial protein nanowires. Scientific Reports, 2016, 6, 23517.	3.3	92
22	Effect of dimerization on the mechanism of action of aurein 1.2. Biochimica Et Biophysica Acta - Biomembranes, 2016, 1858, 1129-1138.	2.6	16
23	Capacitive DNA Detection Driven by Electronic Charge Fluctuations in a Graphene Nanopore. Physical Review Applied, 2015, 3, .	3.8	60
24	Theoretical assessment of feasibility to sequence DNA through interlayer electronic tunneling transport at aligned nanopores in bilayer graphene. Scientific Reports, 2015, 5, 17560.	3.3	45
25	Structural and functional insights into the conductive pili of Geobacter sulfurreducens revealed in molecular dynamics simulations. Physical Chemistry Chemical Physics, 2015, 17, 22217-22226.	2.8	85
26	Unravelling the reaction mechanism of matrix metalloproteinase 3 using QM/MM calculations. Journal of Molecular Structure, 2015, 1091, 125-132.	3.6	10
27	Capacitance spectroscopy and density functional theory. Physical Chemistry Chemical Physics, 2015, 17, 9375-9382.	2.8	45
28	Semi-Empirical Quantum Chemistry Method for Pre-Polymerization Rational Design of Ciprofloxacin Imprinted Polymer and Adsorption Studies. Journal of the Brazilian Chemical Society, 2015, , .	0.6	8
29	Experimental and Theoretical Studies of Volatile Corrosion Inhibitors Adsorption on Zinc Electrode. Journal of the Brazilian Chemical Society, 2014, , .	0.6	3
30	Molecular and Electronic Structure of the Peptide Subunit of Geobacter sulfurreducens Conductive Pili from First Principles. Journal of Physical Chemistry A, 2012, 116, 8023-8030.	2.5	58