Gustavo T Troiano Feliciano

List of Publications by Year
in descending order

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	Thermally activated charge transport in microbial protein nanowires. Scientific Reports, 2016, 6, 23517.	3.3	92
2	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
3	Capacitive DNA Detection Driven by Electronic Charge Fluctuations in a Graphene Nanopore. Physical Review Applied, 2015, 3, .	3.8	60
4	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
5	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
6	Capacitance spectroscopy and density functional theory. Physical Chemistry Chemical Physics, 2015, 17, 9375-9382.	2.8	45
7	Mapping the ionic fingerprints of molecular monolayers. Physical Chemistry Chemical Physics, 2017, 19, 15098-15109.	2.8	22
8	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
9	The role of water on the electronic transport in graphene nanogap devices designed for DNA sequencing. Carbon, 2020, 158, 314-319.	10.3	17
10	Effect of dimerization on the mechanism of action of aurein 1.2. Biochimica Et Biophysica Acta - Biomembranes, 2016, 1858, 1129-1138.	2.6	16
11	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
12	Development of a biomimetic sensor for selective identification of cyanide. Analytical Methods, 2016, 8, 6353-6360.	2.7	11
13	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
14	Unravelling the reaction mechanism of matrix metalloproteinase 3 using QM/MM calculations. Journal of Molecular Structure, 2015, 1091, 125-132.	3.6	10
15	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
16	The density-of-States and equilibrium charge dynamics of redox-active switches. Electrochimica Acta, 2021, 387, 138410.	5.2	8
17	Three-dimensional catalysis and the efficient bioelectrocatalysis beyond surface chemistry. Journal of Catalysis, 2021, 401, 200-205.	6.2	8
18	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

#	Article	IF	Citations
19	Ab Initio QM/MM Simulation of Ferrocene Homogeneous Electron-Transfer Reaction. Journal of Physical Chemistry A, 2021, 125, 25-33.	2.5	7
20	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
21	Simulating DNA Chip Design Using All-Electronic Graphene-Based Substrates. Molecules, 2019, 24, 951.	3.8	6
22	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
23	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
24	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
25	Experimental and Theoretical Studies of Volatile Corrosion Inhibitors Adsorption on Zinc Electrode. Journal of the Brazilian Chemical Society, 2014, , .	0.6	3
26	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
27	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
28	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
29	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
30	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