F Javier Torres

List of Publications by Year in descending order

61 papers	1,007 citations	623734 14 h-index	434195 31 g-index
63 all docs	63 docs citations	63 times ranked	1202 citing authors

#	Article	IF	Citations
1	Naâ‹¯B bond in NaBH: An induced spinâ€polarized bond. ChemPhysChem, 2022, 23, .	2.1	2
2	Dopamine Adsorption on Rutile TiO‹sub›2‹/sub›(110): Geometry, Thermodynamics, and Core-Level Shifts from First Principles. ACS Omega, 2022, 7, 4185-4193.	3.5	3
3	Comparative study of SARS-CoV-2 infection in different cell types: Biophysical-computational approach to the role of potential receptors. Computers in Biology and Medicine, 2022, 142, 105245.	7.0	3
4	Propagation and Parametric Amplification in Four-Wave Mixing Processes: Intramolecular Coupling and High-Order Effects. Symmetry, 2022, 14, 301.	2.2	0
5	Unveiling the structureâ€reactivity relationship involved in the reaction mechanism of the ‹scp›HCl‹/scp›â€catalyzed alkyl ‹i›t‹/i›â€butyl ethers thermal decomposition. A computational study. International Journal of Quantum Chemistry, 2022, 122, .	2.0	2
6	Analysis of Ecuador's SCOPUS scientific production during the 2001â€“2020 period by means of standardized citation indicators. Heliyon, 2022, 8, e09329.	3.2	2
7	Interaction of the New Inhibitor Paxlovid (PF-07321332) and Ivermectin With the Monomer of the Main Protease SARS-CoV-2: A Volumetric Study Based on Molecular Dynamics, Elastic Networks, Classical Thermodynamics and SPT. Computational Biology and Chemistry, 2022, , 107692.	2.3	1
8	A kinetic model for the equilibrium dynamics of absorption and scattering processes in four-wave mixing spectroscopy. AIP Advances, 2022, 12, 065322.	1.3	0
9	A Theoretical and Experimental Study on the Potential Luminescent and Biological Activities of Diaminodicyanoquinodimethane Derivatives. International Journal of Molecular Sciences, 2021, 22, 446.	4.1	2
10	A computational study of the reaction mechanism involved in the fast cleavage of an unconstrained amide bond assisted by an amine intramolecular nucleophilic attack. Journal of Computational Chemistry, 2021, 42, 818-826.	3.3	5
11	Effect of the Nucleophileâ€™s Nature on Chloroacetanilide Herbicides Cleavage Reaction Mechanism. A DFT Study. International Journal of Molecular Sciences, 2021, 22, 6876.	4.1	3
12	When global and local molecular descriptors are more than the sum of its parts: Simple, But Not Simpler?. Molecular Diversity, 2020, 24, 913-932.	3.9	10
13	A valence bond perspective of the reaction force formalism. Theoretical Chemistry Accounts, 2020, 139, 1.	1.4	4
14	Comparative study of the nucleophilic attack step in the proteases catalytic activity: A theoretical study. Molecular Physics, 2020, 118, e1705412.	1.7	5
15	Shannon Entropy and Fisher Information from a Non-Bornâ€“Oppenheimer Perspective. Journal of Physical Chemistry A, 2020, 124, 386-394.	2.5	8
16	A topological study of the haxacoordinated carbon in the pentagonal-pyramidal benzene and hexamethylbenzene dications. Chemical Physics Letters, 2020, 758, 137912.	2.6	5
17	Theoretical Description of Râ€“Xâ‹¯NH3 Halogen Bond Complexes: Effect of the R Group on the Complex Stability and Sigma-Hole Electron Depletion. Molecules, 2020, 25, 530.	3.8	5
18	A review on the information content of the pair density as a tool for the description of the electronic properties in molecular systems. International Journal of Quantum Chemistry, 2019, 119, e25763.	2.0	8

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19	Tensor Algebra-based Geometrical (3D) Biomacro-Molecular Descriptors for Protein Research: Theory, Applications and Comparison with other Methods. Scientific Reports, 2019, 9, 11391.	3.3	7
20	Stability of â€œNo-Pair Ferromagneticâ€•Lithium Clusters. Journal of Physical Chemistry A, 2019, 123, 9721-9728.	2.5	3
21	A valence bond study of the activation of methyl halides bonds by electric fields. Journal of Theoretical and Computational Chemistry, 2019, 18, 1950007.	1.8	2
22	Interaction of ZIKV NS5 and STAT2 Explored by Molecular Modeling, Docking, and Simulations Studies. Lecture Notes in Computer Science, 2019, , 165-176.	1.3	0
23	Theoretical Calculations of the Multistep Reaction Mechanism Involved in Asparagine Pyrolysis Supported by Degree of Rate Control and Thermodynamic Control Analyses. Applied Sciences (Switzerland), 2019, 9, 4847.	2.5	3
24	On the separation of the information content of the Fermi and Coulomb holes and their influence on the electronic properties of molecular systems. Molecular Physics, 2019, 117, 610-625.	1.7	4
25	Theoretical study of the furfuryl benzoate and furfuryl acetate pyrolysis. Journal of Physical Organic Chemistry, 2019, 32, e3790.	1.9	4
26	Higher-Order and Mixed Discrete Derivatives such as a Novel Graph- Theoretical Invariant for Generating New Molecular Descriptors. Current Topics in Medicinal Chemistry, 2019, 19, 944-956.	2.1	2
27	Is the Pauli exclusion principle the origin of electron localisation?. Molecular Physics, 2018, 116, 578-587.	1.7	9
28	Theoretical investigation of the mechanism for the reductive dehalogenation of methyl halides mediated by the CoI-based compounds cobalamin and cobaloxime. Journal of Molecular Modeling, 2018, 24, 316.	1.8	8
29	Understanding the role of Zn²⁺ in the hydrolysis of glycylserine: a mechanistic study by using density functional theory. Molecular Physics, 2017, 115, 403-412.	1.7	3
30	Stability of finite subspaces in density functional theory: Application to simple atoms. International Journal of Quantum Chemistry, 2017, 117, e25400.	2.0	2
31	Discovering key residues of dengue virus NS2b-NS3-protease: New binding sites for antiviral inhibitors design. Biochemical and Biophysical Research Communications, 2017, 492, 631-642.	2.1	12
32	Theoretical analysis of Câ€“F bond cleavage mediated by cob[I]alamin-based structures. Journal of Molecular Modeling, 2017, 23, 264.	1.8	6
33	An alternative description of aromaticity in metallabenzenes. Journal of the Mexican Chemical Society, 2017, 61, .	0.6	1
34	Physico-Chemical and Structural Interpretation of Discrete Derivative Indices on N-Tuples Atoms. International Journal of Molecular Sciences, 2016, 17, 812.	4.1	7
35	The electron localization as the information content of the conditional pair density. Journal of Chemical Physics, 2016, 144, 244104.	3.0	9
36	Mean residence time by hierarchical clustering analysis. Theoretical Chemistry Accounts, 2016, 135, 1.	1.4	3

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37	On the activation of Ïƒ-bonds by electric fields: A Valence Bond perspective. Chemical Physics, 2016, 477, 1-7.	1.9	29
38	Insights on the aromaticity of imidazolylidene carbenes by means of DFT calculations. Computational and Theoretical Chemistry, 2016, 1094, 108-113.	2.5	0
39	On the thermodynamic stability of the intermolecular association between Lewis acids and Lewis bases: a DFT study. Theoretical Chemistry Accounts, 2016, 135, 1.	1.4	11
40	Generalized Molecular Descriptors Derived From Event-Based Discrete Derivative. Current Pharmaceutical Design, 2016, 22, 5095-5113.	1.9	4
41	Molecular Modelling in MRI Contrast Agents Interacting with Water Molecules: Hierarchical Clustering Method for Molecular Dynamics Data Analysis. Biophysical Journal, 2015, 108, 316a.	0.5	0
42	The information content of the conditional pair probability. Chemical Physics Letters, 2015, 635, 116-119.	2.6	6
43	Theoretical evaluation of metal-functionalized rccc R-pyrogallol[4]arenes as media for molecular hydrogen storage. Computational and Theoretical Chemistry, 2015, 1073, 75-83.	2.5	3
44	A theoretical study of the conformational preference of alkyl- and aryl-substituted pyrogallol[4]arenes and evidence of the accumulation of negative electrostatic potential within the cavity of theirrcccconformers. Molecular Simulation, 2014, 40, 327-334.	2.0	6
45	Non-Bornâ€“Oppenheimer nuclear and electronic densities for a three-particle Hookeâ€“Coulomb model. Computational and Theoretical Chemistry, 2013, 1018, 26-34.	2.5	5
46	Ab initio study of the structural, electronic, and thermodynamic properties of linear perfluorooctane sulfonate (PFOS) and its branched isomers. Chemosphere, 2009, 76, 1143-1149.	8.2	39
47	Response to Comment by Sierra Rayne and Kaya Forest on â€˜â€˜Ab initio study of the structural, electronic, and thermodynamic properties of linear perfluorooctane sulfonate (PFOS) and its branched isomersâ€• [Chemosphere 76 (8) (2009) 1143â€“1149]. Chemosphere, 2009, 77, 1457-1458.	8.2	0
48	Normal Vibrational Analysis of the Syndiotactic Polystyrene s(2/1)2 Helix. Journal of Physical Chemistry B, 2009, 113, 5059-5071.	2.6	78
49	A review of the computational studies of proton- and metal-exchanged chabazites as media for molecular hydrogen storage performed with the CRYSTAL code. International Journal of Hydrogen Energy, 2008, 33, 746-754.	7.1	20
50	Ab initio simulation of the IR spectra of pyrope, grossular, and andradite. Journal of Computational Chemistry, 2008, 29, 2268-2278.	3.3	84
51	Hydrogen release from solid state NaBH4. International Journal of Hydrogen Energy, 2008, 33, 3111-3115.	7.1	128
52	Ab Initioinvestigation of the interaction of H₂with lithium exchanged low-silica chabazites. Journal of Physics: Conference Series, 2008, 117, 012012.	0.4	3
53	Thermodynamic and ab initio investigation of the Alâ€“Hâ€“Mg system. Calphad: Computer Coupling of Phase Diagrams and Thermochemistry, 2007, 31, 457-467.	1.6	27
54	Uniplanar Orientations as a Tool To Assign Vibrational Modes of Polymer Chain. Macromolecules, 2007, 40, 3895-3897.	4.8	33

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55	Interaction of H2with Alkali-Metal-Exchanged Zeolites:â€‰ a Quantum Mechanical Study. Journal of Physical Chemistry C, 2007, 111, 2505-2513.	3.1	47
56	Normal Vibrational Analysis of a trans-Planar Syndiotactic Polystyrene Chain. Journal of Physical Chemistry B, 2007, 111, 6327-6335.	2.6	47
57	Theoretical Study of Molecular Hydrogen Adsorption in Mg-Exchanged Chabazite. Journal of Physical Chemistry C, 2007, 111, 1871-1873.	3.1	34
58	An Ab Initio Periodic Study of Acidic Chabazite as a Candidate for Dihydrogen Storage. Journal of Physical Chemistry B, 2006, 110, 10467-10474.	2.6	23
59	Vibrational Spectrum of Katoite Ca3Al2[(OH)4]3:Â A Periodic ab Initio Study. Journal of Physical Chemistry B, 2006, 110, 692-701.	2.6	53
60	Ethanol adsorption on SrTiO3 surfaces. International Journal of Quantum Chemistry, 2006, 106, 1715-1719.	2.0	6
61	Ab InitioStudy of the Vibrational Spectrum and Related Properties of Crystalline Compounds; the Case of CaCO3Calcite. Zeitschrift Fur Physikalische Chemie, 2006, 220, 893-912.	2.8	168