

# F Javier Torres

## List of Publications by Year in descending order

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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	Ab Initio Study of the Vibrational Spectrum and Related Properties of Crystalline Compounds; the Case of CaCO <sub>3</sub> Calcite. <i>Zeitschrift Fur Physikalische Chemie</i> , 2006, 220, 893-912.	2.8	168
2	Hydrogen release from solid state NaBH <sub>4</sub> . <i>International Journal of Hydrogen Energy</i> , 2008, 33, 3111-3115.	7.1	128
3	Ab initio simulation of the IR spectra of pyrope, grossular, and andradite. <i>Journal of Computational Chemistry</i> , 2008, 29, 2268-2278.	3.3	84
4	Normal Vibrational Analysis of the Syndiotactic Polystyrene $s(2/1)_2$ Helix. <i>Journal of Physical Chemistry B</i> , 2009, 113, 5059-5071.	2.6	78
5	Vibrational Spectrum of Katoite Ca <sub>3</sub> Al <sub>2</sub> [(OH) <sub>4</sub> ] <sub>3</sub> : A Periodic ab Initio Study. <i>Journal of Physical Chemistry B</i> , 2006, 110, 692-701.	2.6	53
6	Interaction of H <sub>2</sub> with Alkali-Metal-Exchanged Zeolites: a Quantum Mechanical Study. <i>Journal of Physical Chemistry C</i> , 2007, 111, 2505-2513.	3.1	47
7	Normal Vibrational Analysis of a trans-Planar Syndiotactic Polystyrene Chain. <i>Journal of Physical Chemistry B</i> , 2007, 111, 6327-6335.	2.6	47
8	Ab initio study of the structural, electronic, and thermodynamic properties of linear perfluorooctane sulfonate (PFOS) and its branched isomers. <i>Chemosphere</i> , 2009, 76, 1143-1149.	8.2	39
9	Theoretical Study of Molecular Hydrogen Adsorption in Mg-Exchanged Chabazite. <i>Journal of Physical Chemistry C</i> , 2007, 111, 1871-1873.	3.1	34
10	Uniplanar Orientations as a Tool To Assign Vibrational Modes of Polymer Chain. <i>Macromolecules</i> , 2007, 40, 3895-3897.	4.8	33
11	On the activation of $\sigma$ -bonds by electric fields: A Valence Bond perspective. <i>Chemical Physics</i> , 2016, 477, 1-7.	1.9	29
12	Thermodynamic and ab initio investigation of the Al-H-Mg system. <i>Calphad: Computer Coupling of Phase Diagrams and Thermochemistry</i> , 2007, 31, 457-467.	1.6	27
13	An Ab Initio Periodic Study of Acidic Chabazite as a Candidate for Dihydrogen Storage. <i>Journal of Physical Chemistry B</i> , 2006, 110, 10467-10474.	2.6	23
14	A review of the computational studies of proton- and metal-exchanged chabazites as media for molecular hydrogen storage performed with the CRYSTAL code. <i>International Journal of Hydrogen Energy</i> , 2008, 33, 746-754.	7.1	20
15	Discovering key residues of dengue virus NS2b-NS3-protease: New binding sites for antiviral inhibitors design. <i>Biochemical and Biophysical Research Communications</i> , 2017, 492, 631-642.	2.1	12
16	On the thermodynamic stability of the intermolecular association between Lewis acids and Lewis bases: a DFT study. <i>Theoretical Chemistry Accounts</i> , 2016, 135, 1.	1.4	11
17	When global and local molecular descriptors are more than the sum of its parts: Simple, But Not Simpler?. <i>Molecular Diversity</i> , 2020, 24, 913-932.	3.9	10
18	The electron localization as the information content of the conditional pair density. <i>Journal of Chemical Physics</i> , 2016, 144, 244104.	3.0	9

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19	Is the Pauli exclusion principle the origin of electron localisation?. <i>Molecular Physics</i> , 2018, 116, 578-587.	1.7	9
20	Theoretical investigation of the mechanism for the reductive dehalogenation of methyl halides mediated by the CoI-based compounds cobalamin and cobaloxime. <i>Journal of Molecular Modeling</i> , 2018, 24, 316.	1.8	8
21	A review on the information content of the pair density as a tool for the description of the electronic properties in molecular systems. <i>International Journal of Quantum Chemistry</i> , 2019, 119, e25763.	2.0	8
22	Shannon Entropy and Fisher Information from a Non-Born-Oppenheimer Perspective. <i>Journal of Physical Chemistry A</i> , 2020, 124, 386-394.	2.5	8
23	Physico-Chemical and Structural Interpretation of Discrete Derivative Indices on N-Tuples Atoms. <i>International Journal of Molecular Sciences</i> , 2016, 17, 812.	4.1	7
24	Tensor Algebra-based Geometrical (3D) Biomacro-Molecular Descriptors for Protein Research: Theory, Applications and Comparison with other Methods. <i>Scientific Reports</i> , 2019, 9, 11391.	3.3	7
25	Ethanol adsorption on SrTiO <sub>3</sub> surfaces. <i>International Journal of Quantum Chemistry</i> , 2006, 106, 1715-1719.	2.0	6
26	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 their ccc conformers. <i>Molecular Simulation</i> , 2014, 40, 327-334.	2.0	6
27	The information content of the conditional pair probability. <i>Chemical Physics Letters</i> , 2015, 635, 116-119.	2.6	6
28	Theoretical analysis of C-F bond cleavage mediated by cobalamin-based structures. <i>Journal of Molecular Modeling</i> , 2017, 23, 264.	1.8	6
29	Non-Born-Oppenheimer nuclear and electronic densities for a three-particle Hooke-Coulomb model. <i>Computational and Theoretical Chemistry</i> , 2013, 1018, 26-34.	2.5	5
30	Comparative study of the nucleophilic attack step in the proteases catalytic activity: A theoretical study. <i>Molecular Physics</i> , 2020, 118, e1705412.	1.7	5
31	A topological study of the hexacoordinated carbon in the pentagonal-pyramidal benzene and hexamethylbenzene dications. <i>Chemical Physics Letters</i> , 2020, 758, 137912.	2.6	5
32	Theoretical Description of X-NH <sub>3</sub> Halogen Bond Complexes: Effect of the R Group on the Complex Stability and Sigma-Hole Electron Depletion. <i>Molecules</i> , 2020, 25, 530.	3.8	5
33	A computational study of the reaction mechanism involved in the fast cleavage of an unconstrained amide bond assisted by an amine intramolecular nucleophilic attack. <i>Journal of Computational Chemistry</i> , 2021, 42, 818-826.	3.3	5
34	On the separation of the information content of the Fermi and Coulomb holes and their influence on the electronic properties of molecular systems. <i>Molecular Physics</i> , 2019, 117, 610-625.	1.7	4
35	Theoretical study of the furfuryl benzoate and furfuryl acetate pyrolysis. <i>Journal of Physical Organic Chemistry</i> , 2019, 32, e3790.	1.9	4
36	A valence bond perspective of the reaction force formalism. <i>Theoretical Chemistry Accounts</i> , 2020, 139, 1.	1.4	4

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37	Generalized Molecular Descriptors Derived From Event-Based Discrete Derivative. <i>Current Pharmaceutical Design</i> , 2016, 22, 5095-5113.	1.9	4
38	Ab Initio investigation of the interaction of H <sub>2</sub> with lithium exchanged low-silica chabazites. <i>Journal of Physics: Conference Series</i> , 2008, 117, 012012.	0.4	3
39	Theoretical evaluation of metal-functionalized rccc R-pyrogallol[4]arenes as media for molecular hydrogen storage. <i>Computational and Theoretical Chemistry</i> , 2015, 1073, 75-83.	2.5	3
40	Mean residence time by hierarchical clustering analysis. <i>Theoretical Chemistry Accounts</i> , 2016, 135, 1.	1.4	3
41	Understanding the role of Zn <sup>2+</sup> in the hydrolysis of glycylserine: a mechanistic study by using density functional theory. <i>Molecular Physics</i> , 2017, 115, 403-412.	1.7	3
42	Stability of $\sigma$ -No-Pair Ferromagnetic Lithium Clusters. <i>Journal of Physical Chemistry A</i> , 2019, 123, 9721-9728.	2.5	3
43	Theoretical Calculations of the Multistep Reaction Mechanism Involved in Asparagine Pyrolysis Supported by Degree of Rate Control and Thermodynamic Control Analyses. <i>Applied Sciences (Switzerland)</i> , 2019, 9, 4847.	2.5	3
44	Effect of the Nucleophile's Nature on Chloroacetanilide Herbicides Cleavage Reaction Mechanism. A DFT Study. <i>International Journal of Molecular Sciences</i> , 2021, 22, 6876.	4.1	3
45	Dopamine Adsorption on Rutile TiO <sub>2</sub> (110): Geometry, Thermodynamics, and Core-Level Shifts from First Principles. <i>ACS Omega</i> , 2022, 7, 4185-4193.	3.5	3
46	Comparative study of SARS-CoV-2 infection in different cell types: Biophysical-computational approach to the role of potential receptors. <i>Computers in Biology and Medicine</i> , 2022, 142, 105245.	7.0	3
47	Stability of finite subspaces in density functional theory: Application to simple atoms. <i>International Journal of Quantum Chemistry</i> , 2017, 117, e25400.	2.0	2
48	A valence bond study of the activation of methyl halides bonds by electric fields. <i>Journal of Theoretical and Computational Chemistry</i> , 2019, 18, 1950007.	1.8	2
49	A Theoretical and Experimental Study on the Potential Luminescent and Biological Activities of Diaminodicyanoquinodimethane Derivatives. <i>International Journal of Molecular Sciences</i> , 2021, 22, 446.	4.1	2
50	Higher-Order and Mixed Discrete Derivatives such as a Novel Graph- Theoretical Invariant for Generating New Molecular Descriptors. <i>Current Topics in Medicinal Chemistry</i> , 2019, 19, 944-956.	2.1	2
51	Na $\sigma$ B bond in NaBH: An induced spin-polarized bond. <i>ChemPhysChem</i> , 2022, 23, .	2.1	2
52	Unveiling the structure-reactivity relationship involved in the reaction mechanism of the HCl-catalyzed alkyl <i>tert</i> -butyl ethers thermal decomposition. A computational study. <i>International Journal of Quantum Chemistry</i> , 2022, 122, .	2.0	2
53	Analysis of Ecuador's SCOPUS scientific production during the 2001-2020 period by means of standardized citation indicators. <i>Heliyon</i> , 2022, 8, e09329.	3.2	2
54	An alternative description of aromaticity in metallabenzene. <i>Journal of the Mexican Chemical Society</i> , 2017, 61, .	0.6	1

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55	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. <i>Computational Biology and Chemistry</i> , 2022, , 107692.	2.3	1
56	Response to Comment by Sierra Rayne and Kaya Forest on "Ab initio study of the structural, electronic, and thermodynamic properties of linear perfluorooctane sulfonate (PFOS) and its branched isomers" [Chemosphere 76 (8) (2009) 1143-1149]. <i>Chemosphere</i> , 2009, 77, 1457-1458.	8.2	0
57	Molecular Modelling in MRI Contrast Agents Interacting with Water Molecules: Hierarchical Clustering Method for Molecular Dynamics Data Analysis. <i>Biophysical Journal</i> , 2015, 108, 316a.	0.5	0
58	Insights on the aromaticity of imidazolylidene carbenes by means of DFT calculations. <i>Computational and Theoretical Chemistry</i> , 2016, 1094, 108-113.	2.5	0
59	Interaction of ZIKV NS5 and STAT2 Explored by Molecular Modeling, Docking, and Simulations Studies. <i>Lecture Notes in Computer Science</i> , 2019, , 165-176.	1.3	0
60	Propagation and Parametric Amplification in Four-Wave Mixing Processes: Intramolecular Coupling and High-Order Effects. <i>Symmetry</i> , 2022, 14, 301.	2.2	0
61	A kinetic model for the equilibrium dynamics of absorption and scattering processes in four-wave mixing spectroscopy. <i>AIP Advances</i> , 2022, 12, 065322.	1.3	0