Xavier Fradera

List of Publications by Year
in descending order

26 papers	1,979 citations	516215 16 h-index	610482 24 g-index
27 all docs	27 docs citations	27 times ranked	1477 citing authors

#	Article	IF	Citations
1	Quantitative assessment of the effect of basis set superposition error on the electron density of molecular complexes by means of quantum molecular similarity measures. International Journal of Quantum Chemistry, 2009, 109, 2572-2580.	1.0	0
2	Incorporating protein flexibility into docking and structure-based drug design. Expert Opinion on Drug Discovery, 2006, 1, 335-349.	2.5	30
3	Unsupervised guided docking of covalently bound ligands. Journal of Computer-Aided Molecular Design, 2004, 18, 635-650.	1.3	18
4	Second-order atomic Fukui indices from the electron-pair density in the framework of the atoms in molecules theory. Journal of Computational Chemistry, 2004, 25, 439-446.	1.5	13
5	Guided Docking Approaches to Structure-Based Design and Screening. Current Topics in Medicinal Chemistry, 2004, 4, 687-700.	1.0	62
6	An Insight into the Local Aromaticities of Polycyclic Aromatic Hydrocarbons and Fullerenes.. ChemInform, 2003, 34, no.	0.1	0
7	An Insight into the Local Aromaticities of Polycyclic Aromatic Hydrocarbons and Fullerenes. Chemistry - A European Journal, 2003, 9, 1113-1122.	1.7	125
8	Electron pairing analysis of the Fischer-type chromiumâ€“carbene complexes (CO)5Crĩ...C(X)R (X=H, OH,) Tj ETQq0 0 0 rgBT /Overlock	0.9	18
9	Ligand-induced changes in the binding sites of proteins. Bioinformatics, 2002, 18, 939-948.	1.8	46
10	BIELECTRONIC DENSITIES: ANALYSIS AND APPLICATIONS IN MOLECULAR STRUCTURE AND CHEMICAL REACTIVITY. , 2002, , 831-870.		2
11	Electron localization and delocalization in open-shell molecules. Journal of Computational Chemistry, 2002, 23, 1347-1356.	1.5	34
12	The calculation of electron localization and delocalization indices at the Hartree-Fock, density functional and post-Hartree-Fock levels of theory. Theoretical Chemistry Accounts, 2002, 107, 362-371.	0.5	187
13	Electron-pairing analysis from localization and delocalization indices in the framework of the atoms-in-molecules theory. Theoretical Chemistry Accounts, 2002, 108, 214-224.	0.5	175
14	New Insights in Chemical Reactivity by Means of Electron Pairing Analysis. Journal of Physical Chemistry A, 2001, 105, 2052-2063.	1.1	34
15	Effects of Solvation on the Pairing of Electrons in a Series of Simple Molecules and in the Menshutkin Reaction. Journal of Physical Chemistry A, 2001, 105, 6249-6257.	1.1	32
16	Atomic transferability within the exchange-correlation density. Journal of Computational Chemistry, 2000, 21, 1361-1374.	1.5	11
17	Similarity-driven flexible ligand docking. Proteins: Structure, Function and Bioinformatics, 2000, 40, 623-636.	1.5	87
18	Charge-density concentration and electron-electron coalescence density in atoms and molecules. Physical Review A, 2000, 62, .	1.0	7

#	Article	IF	Citations
19	The mapping of the local contributions of Fermi and Coulomb correlation into intracule and extracule density distributions. Journal of Chemical Physics, 2000, 113, 2530-2543.	1.2	9
20	Effect of basis set superposition error on the electron density of molecular complexes. Journal of Chemical Physics, 2000, 112, 10106-10115.	1.2	24
21	Interpretation of Molecular Intracule and Extracule Density Distributions in Terms of Valence Bond Structures:â€‰ Two-Electron Systems and Processes. Journal of Physical Chemistry A, 2000, 104, 8445-8454.	1.1	11
22	Comparative electronic analysis between hydrogen transfers in the CH₄/CH₃⁺, CH₄/CH₃^{Â•}, and CH₄/CH₃⁻ systems: on the electronic nature of the hydrogen (H⁻, H^{Â•}, H⁺) being transferred. II. Analysis of electron-pair interactions from intracule and extracule densities. Canadian Journal of Chemistry, 2000, 78, 328-337.	0.6	5
23	The Lewis Model and Beyond. Journal of Physical Chemistry A, 1999, 103, 304-314.	1.1	944
24	Second-order quantum similarity measures from intracule and extracule densities. Theoretical Chemistry Accounts, 1998, 99, 44-52.	0.5	11
25	The relevance of the Laplacian of intracule and extracule density distributions for analyzing electronâ€“electron interactions in molecules. Journal of Chemical Physics, 1997, 107, 3576-3583.	1.2	28
26	Application of Molecular Quantum Similarity to QSAR. QSAR and Combinatorial Science, 1997, 16, 25-32.	1.4	58