

# Design of Density Functionals by Combining the Method of Moments with the Self-Consistent Field Method: Parametrization for Thermochemistry, Thermochemical Interactions

Journal of Chemical Theory and Computation

2, 364-382

DOI: 10.1021/ct0502763

Citation Report

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#	ARTICLE	IF	CITATIONS
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#	ARTICLE	IF	CITATIONS
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#	ARTICLE	IF	CITATIONS
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1928	Charge-controlled switchable methane adsorption on heteroatom-doped BNNSs. <i>RSC Advances</i> , 2016, 6, 5079-5088.	3.6	18
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1975	Influence of structural characteristics of substituents on the antioxidant activity of some anthraquinone derivatives. Computational and Theoretical Chemistry, 2016, 1077, 25-31.	2.5	27
1976	The 2H <sup>+</sup> /2e <sup>-</sup> free radical scavenging mechanisms of uric acid: thermodynamics of NH bond cleavage. Computational and Theoretical Chemistry, 2016, 1077, 2-10.	2.5	22
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1999	Predicting the redox properties of uranyl complexes using electronic structure calculations. <i>International Journal of Quantum Chemistry</i> , 2017, 117, e25370.	2.0	9
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2001	Fenamic acid crystal with two asymmetric units ( $Z' = 2$ ): why $Z' = 2$ rather than $Z' = 1$ . <i>CrystEngComm</i> , 2017, 19, 1762-1770.	2.6	14
2002	Understanding photophysical properties of chiral conjugated corrals for organic photovoltaics. <i>Journal of Materials Chemistry C</i> , 2017, 5, 3495-3502.	5.5	10
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2005	Theoretical and experimental study on the degradation mechanism of atrazine in Fenton oxidation treatment. <i>RSC Advances</i> , 2017, 7, 1581-1587.	3.6	11
2006	A quantum chemical study on the OH radical quenching by natural antioxidant fisetin. <i>Journal of Physical Organic Chemistry</i> , 2017, 30, e3692.	1.9	5
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2008	Phenalenyl $\pi$ -Dimer under the External Electric Field: Two-Electron/12-Center Bonding Breaking and Emergence of Electrostatic Interaction. <i>Journal of Physical Chemistry C</i> , 2017, 121, 3765-3770.	3.1	12
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2011	A quantum chemical study on $\text{E}^{\text{TM}}$ Cl-initiated atmospheric degradation of acrylonitrile. <i>RSC Advances</i> , 2017, 7, 20574-20581.	3.6	3
2012	Investigation of the solvent effect, molecular structure, electronic properties and adsorption mechanism of Tegafur anticancer drug on Graphene nanosheet surface as drug delivery system by molecular dynamics simulation and density functional approach. <i>Journal of Inclusion Phenomena and Macrocyclic Chemistry</i> , 2017, 88, 159-169.	1.6	53
2013	Quantum Chemical Estimation of Acetone Physisorption on Graphene Using Combined Basis Set and Size Extrapolation Schemes. <i>Journal of Physical Chemistry C</i> , 2017, 121, 8999-9010.	3.1	5
2014	Second-order nonlinear optical properties of composite material of an azo-chromophore with a tricyanodiphenyl acceptor in a poly(styrene- co -methyl methacrylate) matrix. <i>Optical Materials</i> , 2017, 69, 67-72.	3.6	9
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#	ARTICLE	IF	CITATIONS
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2089	CO <sub>2</sub> Complexes with Five-Membered Heterocycles: Structure, Topology, and Spectroscopic Characterization. <i>Journal of Physical Chemistry A</i> , 2017, 121, 9118-9130.	2.5	12
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2095	The BioFragment Database (BFDdb): An open-data platform for computational chemistry analysis of noncovalent interactions. <i>Journal of Chemical Physics</i> , 2017, 147, 161727.	3.0	82
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#	ARTICLE	IF	CITATIONS
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#	ARTICLE	IF	CITATIONS
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#	ARTICLE	IF	CITATIONS
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