

# Damian Moran

## List of Publications by Year in descending order

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34  
papers

4,307  
citations

236833

25  
h-index

395590

33  
g-index

35  
all docs

35  
docs citations

35  
times ranked

5229  
citing authors

#	ARTICLE	IF	CITATIONS
1	An Evaluation of Harmonic Vibrational Frequency Scale Factors. <i>Journal of Physical Chemistry A</i> , 2007, 111, 11683-11700.	1.1	2,264
2	Popular Theoretical Methods Predict Benzene and Arenes To Be Nonplanar. <i>Journal of the American Chemical Society</i> , 2006, 128, 9342-9343.	6.6	238
3	The oxidation states of copper and iron in mineral sulfides, and the oxides formed on initial exposure of chalcopyrite and bornite to air. <i>Geochimica Et Cosmochimica Acta</i> , 2006, 70, 2210-2228.	1.6	202
4	Towards Graphite: Magnetic Properties of Large Polybenzenoid Hydrocarbons. <i>Journal of the American Chemical Society</i> , 2003, 125, 6746-6752.	6.6	158
5	On the Stability of Large [4n]Annulenes. <i>Organic Letters</i> , 2003, 5, 2983-2986.	2.4	118
6	σ-Antiaromaticity in Cyclobutane, Cubane, and Other Molecules with Saturated Four-Membered Rings. <i>Organic Letters</i> , 2003, 5, 23-26.	2.4	108
7	Bond Dissociation Energies and Radical Stabilization Energies: An Assessment of Contemporary Theoretical Procedures. <i>Journal of Physical Chemistry A</i> , 2007, 111, 13638-13644.	1.1	101
8	Aromaticity of the Bergman, Myers-Saito, Schmittel, and Directly Related Cyclizations of Ene-diyne. <i>Journal of Organic Chemistry</i> , 2002, 67, 1453-1461.	1.7	80
9	2-Pyridinethiol/2-Pyridinethione Tautomeric Equilibrium. A Comparative Experimental and Computational Study. <i>Journal of Organic Chemistry</i> , 2002, 67, 9061-9069.	1.7	78
10	Bond Dissociation Energies and Radical Stabilization Energies Associated with Model Peptide-Backbone Radicals. <i>Journal of Physical Chemistry A</i> , 2005, 109, 6318-6325.	1.1	72
11	An Assessment of Theoretical Procedures for Predicting the Thermochemistry and Kinetics of Hydrogen Abstraction by Methyl Radical from Benzene. <i>Journal of Physical Chemistry A</i> , 2006, 110, 8942-8951.	1.1	70
12	Structures, Stabilities, and Ionization Potentials of Dodecahedrane Endohedral Complexes. <i>Journal of Physical Chemistry A</i> , 2002, 106, 5144-5154.	1.1	64
13	Metal-Mediated Formation of Gas-Phase Amino Acid Radical Cations. <i>Journal of Physical Chemistry A</i> , 2006, 110, 8304-8315.	1.1	64
14	σ-Aromaticity and σ-Antiaromaticity in Saturated Inorganic Rings. <i>Journal of Physical Chemistry A</i> , 2005, 109, 3711-3716.	1.1	60
15	An Experimental and Theoretical Investigation of Gas-Phase Reactions of Ca <sup>2+</sup> with Glycine. <i>Chemistry - A European Journal</i> , 2006, 12, 6787-6796.	1.7	57
16	Carbene Stabilization by Aryl Substituents. Is Bigger Better?. <i>Journal of the American Chemical Society</i> , 2007, 129, 3763-3770.	6.6	56
17	Gas-phase regiocontrolled generation of charged amino acid and peptide radicals. <i>Chemical Communications</i> , 2006, , 4233.	2.2	52
18	Ab Initio Modeling of Glycosyl Torsions and Anomeric Effects in a Model Carbohydrate: 2-Ethoxy Tetrahydropyran. <i>Biophysical Journal</i> , 2007, 93, 1-10.	0.2	48

#	ARTICLE	IF	CITATIONS
19	On the Viability of Small Endohedral Hydrocarbon Cage Complexes: $X@C_4H_4$ , $X@C_8H_8$ , $X@C_8H_{14}$ , $X@C_{10}H_{16}$ , $X@C_{12}H_{12}$ , and $X@C_{16}H_{16}$ . <i>Journal of the American Chemical Society</i> , 2003, 125, 11442-11451.	6.6	45
20	Structures and Stabilities of Endo- and Exohedral Dodecahedrane Complexes ( $X@C_{20}H_{20}$ and) <i>Tj ETQq0 0 0 rgBT /Overlock 10 Tf 50 70</i>	1.1	42
21	Thermochemistry and Kinetics of Hydrogen Abstraction by Methyl Radical from Polycyclic Aromatic Hydrocarbons. <i>Journal of Physical Chemistry A</i> , 2006, 110, 13624-13631.	1.1	41
22	Rearrangements in Model Peptide-Type Radicals via Intramolecular Hydrogen-Atom Transfer. <i>Helvetica Chimica Acta</i> , 2006, 89, 2254-2272.	1.0	39
23	Aromatic stabilization in heterofullerenes $C_{48}X_{12}$ ( $X = N, P, B, Si$ ). <i>Journal of Physical Organic Chemistry</i> , 2003, 16, 726-730.	0.9	35
24	Intramolecular Diels-Alder Reactions of Ester-Linked 1,3,8-Nonatrienes. <i>Journal of Organic Chemistry</i> , 2005, 70, 5561-5570.	1.7	33
25	Theoretical Study of Icosahedral closo-Borane, -Alane, and -Gallane Dianions ( $A_{12}H_{12}^{2-}$ ; A = B, Al, Ga) with Endohedral Noble Gas Atoms (Ng = He, Ne, Ar, and Kr) and Their Lithium Salts ( $Li[Ng@A_{12}H_{12}]$ -and) <i>Tj ETQq11.10.784317 rgBT</i>	1.1	27
26	The Almost Bottleable Triplet Carbene: $2,6$ -dibromo-4-tert-butyl-2,6-bis(trifluoromethyl)-4-isopropylidiphenylcarbene. <i>Journal of the American Chemical Society</i> , 2001, 123, 4331-4335.	6.6	25
27	Theoretical Study of Complexes of Closo-Borane, Alane, and Gallane Anions with Cations of Light Metals Inside and Outside of Icosahedral Clusters [ $A_{12}H_{12}^-$ ] (A = B, Al, and Ga). <i>Journal of Physical Chemistry A</i> , 2002, 106, 11594-11602.	1.1	23
28	A Theoretical and Structural Investigation of Thiocarbon Anions. <i>Journal of Organic Chemistry</i> , 2003, 68, 8808-8814.	1.7	23
29	On the Origin of Cis/Trans Stereoselectivity in Intramolecular Diels-Alder Reactions of Substituted Pentadienyl Acrylates: A Comprehensive Density Functional Study. <i>Journal of Organic Chemistry</i> , 2005, 70, 10841-10853.	1.7	22
30	Increased Reactivity of the $Cr(CO)_3(C_5Me_5)$ Radical with Thiones versus Thiols: A Theoretical and Experimental Investigation. <i>Inorganic Chemistry</i> , 2003, 42, 8494-8503.	1.9	19
31	Th-Symmetrical $N_8(C_6)$ and $P_8(C_6)$ ; an Extraordinary Contrast in Heterofullerene Stability. <i>Organic Letters</i> , 2001, 3, 3233-3236.	2.4	18
32	Impact of Hydrogen Bonding on the Susceptibility of Peptides to Oxidation. <i>Chemistry - an Asian Journal</i> , 2017, 12, 1485-1489.	1.7	11
33	Molecular structures and energetics of the neutral aluminum-trimethylaluminum complex: an Al-Al bonded global minimum?. <i>Chemical Physics Letters</i> , 2003, 378, 65-70.	1.2	2
34	Theoretical Study of Complexes of Closo-Borane, Alane, and Gallane Anions with Cations of Light Metals Inside and Outside of Icosahedral Clusters [ $A_{12}H_{12}^-$ ] (A: B, Al, and Ga).. <i>ChemInform</i> , 2003, 34, no.	0.1	0