Aristides Mavridis

List of Publications by Year
in descending order

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129	2,528	201385	288905
papers	citations	27 h-index	40 g-index

137	137	137	1562
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	An accurate description of the ground and excited states of CH. Journal of Chemical Physics, 1999, 111, 9536-9548.	1.2	99
2	Theoretical investigation of iron carbide, FeC. Journal of Chemical Physics, 2002, 116, 4901.	1.2	75
3	Electronic Structure and Bonding of the Early 3d-Transition Metal Diatomic Oxides and Their Ions: ScO^{0,Â±}, TiO^{0,Â±}, CrO^{0,Â±}, and MnO^{0,Â±}^{â€}. Journal of Physical Chemistry A, 2010, 114, 8536-8572.	1.1	72
4	Carbonyl Boron and Related Systems:â€‰ An ab Initio Study of Bâ^'X and YBâ‹®BY (1Î£g+), Where X = He, Ne, Ar, Kr, CO, CS, N2 and Y = Ar, Kr, CO, CS, N2. Journal of Physical Chemistry A, 2004, 108, 4335-4340.	1.1	66
5	Electronic Structure of Vanadium Oxide. Neutral and Charged Species, VO0,Â±. Journal of Physical Chemistry A, 2007, 111, 1953-1965.	1.1	65
6	On the dipole moment of the ground state Xâ€Š3Î" of iron carbide, FeC. Journal of Chemical Physics, 2003, 118, 4984-4986.	1.2	63
7	First principles study of the ground and excited states of FeO, FeO+, and FeOâ^'. Journal of Chemical Physics, 2011, 134, 234308.	1.2	63
8	Electronic structure and bonding of ozone. Journal of Chemical Physics, 2008, 129, 054312.	1.2	56
9	First principles study of the electronic structure and bonding of Mn2. Journal of Chemical Physics, 2008, 129, 154310.	1.2	51
10	First Principles Examination of the Acetyleneâ^'Water Clusters, HCCHâ^'(H2O)x,x= 2, 3, and 4. Journal of Physical Chemistry A, 2002, 106, 11327-11337.	1.1	49
11	CH2 revisited. Canadian Journal of Chemistry, 2004, 82, 684-693.	0.6	49
12	Asymmetrical changes in the tertiary structure of Î±-chymotrypsin with change in pH. Biochemistry, 1974, 13, 3661-3666.	1.2	47
13	Theoretical Investigation of Scandium Carbide, ScC. Journal of Physical Chemistry A, 2001, 105, 755-759.	1.1	45
14	On the electrostatic bonding of carbonyl to the monocations of the first-row transition elements. Journal of the American Chemical Society, 1989, 111, 2482-2487.	6.6	44
15	Electronic structure and bonding of the 3d transition metal borides, MB, M=Sc, Ti, V, Cr, Mn, Fe, Co, Ni, and Cu through all electron ab initio calculations. Journal of Chemical Physics, 2008, 128, 034309.	1.2	41
16	Interaction of Dioxygen with Al Clusters and Al(111):â€‰ A Comparative Theoretical Study. Journal of Physical Chemistry C, 2008, 112, 6924-6932.	1.5	41
17	On the ground states of CaC and ZnC: A multireference Brillouinâ€"Wigner coupled cluster study. Journal of Chemical Physics, 2002, 117, 9733-9739.	1.2	40
18	First-Principles Investigation of the Boron and Aluminum Carbides BC and AlC and Their Anions BC-and AlC-. 1. Journal of Physical Chemistry A, 2001, 105, 1175-1184.	1.1	39

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19	The dissociation energies of NF(Xâ€‰3Î£â^) and NCl(Xâ€‰3Î£â^). Journal of Chemical Physics, 1997, 106, 3280-3286.	1.2	36
20	A Multireference Coupled-Cluster Potential Energy Surface of Diazomethane, CH2N2. Journal of Physical Chemistry A, 2005, 109, 10148-10152.	1.1	35
21	A first principles study of the acetyleneâ€“water interaction. Journal of Chemical Physics, 2000, 112, 6178-6189.	1.2	34
22	Ab initio investigation of the ground and low-lying states of the diatomic fluorides TiF, VF, CrF, and MnF. Journal of Chemical Physics, 2004, 120, 11500-11521.	1.2	34
23	Theoretical Investigation of Titanium Carbide, TiC:â€‰ X3Î£+, aÎ£+, A3Î”, and b1Î” States. Journal of Physical Chemistry A, 2002, 106, 3905-3908.	1.1	30
24	On the Bonding Nature of the N5+(=N(N2)2+) Cation and Related Species N(CO)x+, N(NH3)x+, and NRx+, x = 1, 2 and R = He, Ne, Ar, Kr. Do We Really Need the Resonance Concept?. Journal of Physical Chemistry A, 2002, 106, 4435-4442.	1.1	30
25	The electronic structure of vanadium carbide, VC. Journal of Chemical Physics, 2005, 123, 014301.	1.2	28
26	Ab initio investigation of the electronic structure and bonding of BH, BHâ^', and HBBH molecules. Journal of Chemical Physics, 2008, 128, 144308.	1.2	28
27	The Sc2 dimer revisited. Journal of Chemical Physics, 2010, 132, 024309.	1.2	28
28	Theoretical Study of the Electronic and Geometrical Structure of the Ground and Low-Lying States of NCl2, PCl2, NCl, and PCl Radicals. The Journal of Physical Chemistry, 1995, 99, 10759-10765.	2.9	27
29	An accurate description of the ground and excited states of SiH. Journal of Chemical Physics, 2002, 116, 6529-6540.	1.2	27
30	On symmetry breaking in BNB: Real or artifactual?. Journal of Chemical Physics, 2004, 120, 1813-1819.	1.2	27
31	Electronic Structure of Cobalt Carbide, CoC. Journal of Physical Chemistry A, 2006, 110, 8952-8962.	1.1	26
32	Accurate ab initio calculations of the ground states of FeC, FeC+, and FeCâ^'. Journal of Chemical Physics, 2010, 132, 194312.	1.2	26
33	Ab Initio Investigation of the LiHe X2Î£+, A2Î, and B2Î£+States:Â A Basis Set Study. Journal of Physical Chemistry A, 2000, 104, 408-412.	1.1	25
34	Electronic structure of carbon-lithium, silicon-hydrogen, and silicon-lithium in the lowest 4.SIGMA.- and 2.pi. states. The Journal of Physical Chemistry, 1982, 86, 1979-1985.	2.9	24
35	The gas phase chemistry of bare and ligated transition metal ions: Correlations of reactivity with electronic structureâ€”I. M+ and MCO+. Polyhedron, 1988, 7, 1559-1572.	1.0	24
36	Theoretical investigation of theX2Î£+,A2Î, andB2Î£+ states of LiAr and LiKr. Journal of Chemical Physics, 2002, 116, 9305-9314.	1.2	24

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37	Electronic Structure of Scandium and Titanium Carbide Cations, ScC+and TiC+. Ground and Low-Lying States. Journal of Physical Chemistry A, 2000, 104, 11777-11785.	1.1	23
38	Electronic structure of the carbyne C-Li and the carbene Li2C. Journal of the American Chemical Society, 1982, 104, 3827-3833.	6.6	22
39	A Theoretical Investigation of the Structure and Bonding of Diazomethane, CH2N2. Journal of Physical Chemistry A, 1999, 103, 1255-1259.	1.1	22
40	Accurate Theoretical Study of the Excited States of Boron and Aluminum Carbides, BC, AlC. 2. Journal of Physical Chemistry A, 2001, 105, 7672-7685.	1.1	22
41	Ab Initio Study of the Ground and Excited States of Zinc Carbide, ZnC. Journal of Physical Chemistry A, 2003, 107, 6062-6072.	1.1	22
42	Multireference configuration interaction and coupled-cluster calculations on the X3Î£â¯, a1Î”, and b1Î£+ states of the NF molecule. International Journal of Quantum Chemistry, 2005, 104, 458-467.	1.0	22
43	Ab initio Study of the Diatomic Fluorides FeF, CoF, NiF, and CuF. Journal of Physical Chemistry A, 2008, 112, 11235-11250.	1.1	22
44	Ab initioinvestigation of the ground state properties of PO, PO+, and POâ¯. Journal of Chemical Physics, 2003, 119, 5981-5987.	1.2	21
45	Electronic and geometric structure of the 3d-transition metal monocarbonyls MCO, M=Sc, Ti, V, and Cr. Journal of Chemical Physics, 2005, 123, 074327.	1.2	21
46	First principles study of the diatomic charged fluorides MFÂ±, M=Sc, Ti, V, Cr, and Mn. Journal of Chemical Physics, 2005, 122, 054312.	1.2	21
47	Crystal and molecular structure of dimethoxyporphinato-germanium(IV). Inorganic Chemistry, 1976, 15, 2723-2727.	1.9	20
48	An ab initio study of the electronic structure of the ground triplet and low-lying singlet states of formylnitrene, HCON and formylphosphinidene, HCOP. Journal of the American Chemical Society, 1980, 102, 7651-7655.	6.6	20
49	Ground states of BeC and MgC: A comparative multireference Brillouin-Wigner coupled cluster and configuration interaction study. International Journal of Quantum Chemistry, 2005, 102, 762-774.	1.0	20
50	Theoretical investigation of the ground and low-lying excited states of nickel carbide, NiC. Journal of Chemical Physics, 2007, 126, 194304.	1.2	20
51	Electronic Structure and Bonding of Cobalt Monoxide, CoO, and Its Ions CoO+ and CoOâ€“: An Ab Initio Study. Journal of Physical Chemistry A, 2012, 116, 6935-6949.	1.1	20
52	First principles exploration of NiO and its ions NiO+ and NiOâ¯. Journal of Chemical Physics, 2013, 138, 054308.	1.2	20
53	First principles investigation of chromium carbide, CrC. Journal of Chemical Physics, 2005, 123, 014302.	1.2	19
54	Electronic spectroscopy and electronic structure of diatomic CrC. Journal of Chemical Physics, 2010, 133, 034303.	1.2	19

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55	An Accurate Description of the LiNe X 2Î£+, A 2Î, and B 2Î£+ States. Journal of Physical Chemistry A, 2001, 105, 1983-1987.	1.1	18
56	A molecular level study of the aqueous microsolvation of acetylene. Chemical Physics Letters, 2001, 340, 538-546.	1.2	18
57	The dipole moments of the excited states of FeC. Journal of Chemical Physics, 2005, 122, 056101.	1.2	18
58	On the electron affinity of SiN and spectroscopic constants of SiNâ¯. Journal of Chemical Physics, 2005, 123, 124301.	1.2	18
59	An ab initio study of the electronic structure of BF and BF+. Journal of Chemical Physics, 2013, 138, 104312.	1.2	18
60	Ab initio structural study of the B4H4 molecule. Asymmetric structure for a â€˜symmetricâ€™ system. Chemical Physics Letters, 1994, 226, 469-474.	1.2	17
61	Electronic structure of vanadium and chromium carbide cations, VC+and CrC+. Ground and low-lying states. Molecular Physics, 2004, 102, 2451-2466.	0.8	17
62	First Principles Investigation of the Electronic Structure of the Iron Carbide Cation, FeC+. Journal of Physical Chemistry A, 2005, 109, 9249-9258.	1.1	17
63	Bonding Elucidation of the Three Common Acids H2SO4, HNO3, and HClO4. Journal of Physical Chemistry A, 2009, 113, 13972-13975.	1.1	16
64	An accurate first principles study of the geometric and electronic structure of B2, B2â¯, B3, B3â¯, and B3H: Ground and excited states. Journal of Chemical Physics, 2010, 132, 164307.	1.2	16
65	The electronic structure of Ti2 and Ti2+. Journal of Chemical Physics, 2011, 135, 134302.	1.2	16
66	Ab initio Study of the Electronic Structure of Zinc Oxide and its Ions, ZnO0,Â±. Ground and Excited States. Journal of Physical Chemistry A, 2010, 114, 9333-9341.	1.1	15
67	First-Principles Investigation of the Early 3d Transition Metal Diatomic Chlorides and Their Ions, ScCl0,Â±, TiCl0,Â±, VCl0,Â±, and CrCl0,Â±. Journal of Physical Chemistry A, 2009, 113, 6818-6840.	1.1	14
68	Myths and Reality of Hypervalent Molecules. The Electronic Structure of FClO_x, x = 1â¯3, Cl₃PO, Cl₃PCH₂, Cl₃CClO, and C(ClO)₄. Journal of Physical Chemistry A, 2011, 115, 2378-2384.	1.1	14
69	Electronic Structure of the Ground and Low-Lying Excited States of TiP. The Journal of Physical Chemistry, 1996, 100, 13971-13975.	2.9	13
70	A Theoretical Study of Calcium Monohydride, CaH:â€‰ Low-Lying States and Their Permanent Electric Dipole Moments. Journal of Physical Chemistry A, 2007, 111, 371-374.	1.1	13
71	Electronic and geometric structure of amidoscandium(1+) and amminescandium(1+). The Journal of Physical Chemistry, 1991, 95, 6854-6859.	2.9	12
72	Elucidation of the structural characteristics of the isovalent species Li[CO] and Li[CS] by ab anitio calculations. Chemical Physics Letters, 1996, 259, 185-192.	1.2	12

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73	On the Electronic Structure of ScB+: Ground and Low-Lying Excited States. Advances in Quantum Chemistry, 1998, , 69-91.	0.4	12
74	SiH2, a critical study. Molecular Physics, 2004, 102, 2597-2606.	0.8	12
75	Ab initio study of the electronic structure of manganese carbide. Journal of Chemical Physics, 2006, 124, 154308.	1.2	12
76	First principles study of cobalt hydride, CoH, and its ions CoH+ and CoHâ^'. Journal of Chemical Physics, 2012, 137, 034309.	1.2	12
77	Electronic and geometric structure of the titanium hydrides, TiH+ and TiH + 2. Journal of the Chemical Society, Faraday Transactions 2, 1989, 85, 1391.	1.1	11
78	Electronic and geometrical structure of the NF2 radical. Chemical Physics Letters, 1993, 216, 167-172.	1.2	11
79	Bonding Investigation of the Ground and Low-Lying States of the Titanium Boride Cation, TiB+. Journal of Physical Chemistry A, 1998, 102, 5982-5992.	1.1	11
80	â€œHypervalencyâ€•and the chemical bond. Computational and Theoretical Chemistry, 2019, 1153, 65-74.	1.1	11
81	Ground and Low-Lying States of the Vanadium Boride Cation, VB+:â€‰ An ab Initio Investigation. Journal of Physical Chemistry A, 1999, 103, 3336-3345.	1.1	10
82	Structure and Bonding of the Polytopic Molecule Li[BO]. A Theoretical Investigation. Journal of Physical Chemistry A, 2001, 105, 7106-7110.	1.1	10
83	Electronic structure of linear TiCH. Journal of Chemical Physics, 2003, 119, 3745-3750.	1.2	10
84	Ab Initio Investigation of the Electronic and Geometric Structure of Magnesium Diboride, MgB2. Journal of Physical Chemistry A, 2005, 109, 10663-10674.	1.1	10
85	Structure and Energetics of Gaseous HZnCl. Journal of Physical Chemistry A, 2006, 110, 10899-10903.	1.1	9
86	The electronic structure of the two lowest states of CuC. Journal of Chemical Physics, 2008, 129, 174306.	1.2	9
87	Li atoms attached to helium nanodroplets. International Journal of Quantum Chemistry, 2011, 111, 400-405.	1.0	9
88	Electronic spectroscopy and electronic structure of diatomic TiFe. Journal of Chemical Physics, 2012, 137, 054302.	1.2	9
89	Accurate first principles calculations on chlorine fluoride ClF and its ions ClFÂ±. Theoretical Chemistry Accounts, 2014, 133, 1.	0.5	9
90	Electronic structure of CNa and CNa2 in their electronic ground states. The Journal of Physical Chemistry, 1984, 88, 4973-4978.	2.9	8

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91	On the electronic structure of the ground (X3Î£â¯) and some low-lying excited states (A3Î, a1Î”, b1â¯+, B3Î£â¯) of the isovalent species Pî—¸Li and Pî—¸Na. Computational and Theoretical Chemistry, 1997, 417, 277-287.	1.5	8
92	Electronic structure determination of chromium boride cation, CrB+. Journal of Chemical Physics, 2000, 113, 2270-2281.	1.2	8
93	A highly accurate first principles determination of the electron affinity of BO(X2Î£+) and binding energy of BOâ¯(X1Î£+). Chemical Physics Letters, 2001, 341, 382-386.	1.2	8
94	Theoretical Investigation of Organo-Noble Gas Compounds, HC(Ng)n+,n= 1, 2; Ng = He, Ne, Ar, Kr, and Xe. Evidence for Potentially Isolable HCArn+, HCKrn+, and HCXen+Species. Journal of Physical Chemistry A, 2004, 108, 11127-11131.	1.1	8
95	Ab Initio Study of the Electronic Structure and Bonding of Aluminum Nitride. Journal of Physical Chemistry A, 2007, 111, 11221-11231.	1.1	8
96	All-Electron First Principles Calculations of the Ground and Some Low-Lying Excited States of BaI. Journal of Physical Chemistry A, 2007, 111, 10002-10009.	1.1	8
97	Electronic Structure and Bonding of the Fastidious Species CN₂ and CP₂: A First-Principles Study. Journal of Physical Chemistry A, 2019, 123, 10290-10302.	1.1	8
98	Near-Hartreeâ€“Fock calculations on the ground state of the fluoronium ion, FH+2. Journal of the Chemical Society, Faraday Transactions 2, 1982, 78, 447-455.	1.1	7
99	An ab initio structural study of cyanamide. Computational and Theoretical Chemistry, 1993, 279, 151-156.	1.5	7
100	Ab initio study of the ground and several excited states of the NLi system. Chemical Physics Letters, 1996, 250, 409-414.	1.2	7
101	Theoretical Investigation of the Ground X3Î£- State of Nitrogen Bromide. Journal of Physical Chemistry A, 1998, 102, 10536-10539.	1.1	7
102	Electronic Structure and Bonding Nature of the Ground State Monocarbide Cations, ScC+, TiC+, VC+, and CrC+. Collection of Czechoslovak Chemical Communications, 2003, 68, 387-404.	1.0	7
103	All-Electron ab Initio Calculations on Tetramethyltin. The Journal of Physical Chemistry, 1994, 98, 8906-8909.	2.9	6
104	Electronic and Geometrical Structure of the Sc[BO]+Cation. An Ab Initio Investigation. Journal of Physical Chemistry A, 1999, 103, 9359-9363.	1.1	6
105	Predissociation lifetimes of the E2Î and F2Î states of CH. Chemical Physics Letters, 2000, 331, 89-94.	1.2	6
106	Conditions conducive to the chemi-ionization reaction O(3P)+CH(Xâ€Š2Î,aâ€Š4Î£â¯)â†'HCO+(Xâ€Š1Î£+)+eâ¯. Journal of Chemical Physics, 2001, 115, 6946-6950.	1.2	6
107	On the ground state of titanium phosphide, TiP: A theoretical investigation. Journal of Chemical Physics, 2004, 121, 2646.	1.2	6
108	Structural parameters of the ground states of the quasiâ€stable diatomic anions CO^{â¯}, BF^{â¯}, and BCl^{â¯} as obtained by conventional Ab Initio methods. International Journal of Quantum Chemistry, 2015, 115, 771-778.	1.0	6

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109	The story of the B 4 H 4 molecule told again. Computational and Theoretical Chemistry, 2017, 1115, 217-222.	1.1	6
110	Theoretical Investigation of the Electronic States of Calcium Carbide, CaC. Journal of Physical Chemistry A, 2003, 107, 7650-7655.	1.1	5
111	A theoretical study of the geometrical structure and energy inversion barriers of the cyanopnictogens Nî—¼C-XY2 (X = N or P; Y = H, F, Cl or Br). Computational and Theoretical Chemistry, 1994, 305, 225-239.	1.5	4
112	On the Electronic Structure of NLi2and PLi2, Ground and Low-Lying Excited States. Journal of Physical Chemistry A, 1998, 102, 2223-2230.	1.1	3
113	The Electronic Structure of ScAl+. Ground and Low-Lying Excited States. Journal of Physical Chemistry A, 2000, 104, 6861-6870.	1.1	3
114	CH(X2â^¸a4â^ž) â€¦ OH2 and CH2(??3B1, Ã£1A1) â€¦ OH2 interactions. A first principles investigation. International Journal of Quantum Chemistry, 2005, 104, 497-511.	1.0	3
115	Interaction of the early 3d transition metals Sc, Ti, V, and Cr with N2: An ab initio study. Journal of Chemical Physics, 2006, 124, 104306.	1.2	3
116	Structural characterization of scandium monophosphide (1+). The Journal of Physical Chemistry, 1993, 97, 10955-10957.	2.9	2
117	Ab Initio Investigation of the Electronic Structure and Bonding of the HC(N2)x+ and HC(CO)x+ Cations, x = 1, 2. Journal of Physical Chemistry A, 2005, 109, 6549-6554.	1.1	2
118	Structure and bonding of ScCN and ScNC: Ground and low-lying states. Chemical Physics, 2012, 399, 46-49.	0.9	2
119	All electron ab initio calculations on the ScTi molecule: a really hard nut to crack. Theoretical Chemistry Accounts, 2013, 132, 1.	0.5	2
120	Accurate ab Initio Structural Parameters of the Diatomic and Triatomic van der Waals Molecules ¹¹BNg (X²Î, A²Î£⁺) and ¹¹BNg₂ (XÌƒ²B₁), Ng = ⁴He, ²⁰Ne, ⁴⁰Ar, ⁸⁴Kr, and ¹³²Xe. Journal of Physical Chemistry A, 2014, 118, 3990-3995.	1.1	2
121	An ab initio study of Li+ â€¦Cî—¼S, a purely electrostatic system. Computational and Theoretical Chemistry, 1995, 357, 97-101.	1.5	1
122	The electronic structure and bonding of AlNAl. Journal of Chemical Physics, 2009, 130, 154308.	1.2	1
123	Accurate structural parameters and binding energy of the <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" altimg="si1.gif" overflow="scroll"><mml:mrow><mml:mover accent="true"><mml:mrow><mml:msup><mml:mrow><mml:mi>X</mml:mi></mml:mrow><mml:mrow><mml:mn>1</mml:mn></mml:mrow></mml:msup></mml:mrow></mml:mover></mml:mrow></mml:math> state of diazomethane through. Chemical Physics Letters, 2014, 600, 103-105.	1.2	1
124	A well known quantum theorem revisited. European Journal of Physics, 1990, 11, 152-154.	0.3	0
125	The ScPH+ Cation. The Journal of Physical Chemistry, 1994, 98, 12232-12235.	2.9	0
126	Ab initio Study of the Ground and Excited States of Zinc Carbide, ZnC.. ChemInform, 2003, 34, no.	0.1	0

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127	1937 Nobel Prize. American Journal of Physics, 2006, 74, 373-373.	0.3	0
128	Electronic and Geometric Structure of the 3d-Transition Metal Monocarbonyls MCO, M = Sc, Ti, V and Cr. , 2006, , 1505-1505.		0
129	The Interaction of the Early 3d-transition metals Sc, Ti, V and Cr with N2 . An ab initio Study. , 2006, , 1497-1497.		0