Eugene S Kryachko

List of Publications by Year
in descending order

72	2,062	257101 24	288905 40
papers	citations	h-index	g-index

76	76	76	1580
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	On the Existence of Heï£¿He Bond in the Endohedral Fullerene HÐµ₂@C₆₀. Journal of Computational Chemistry, 2018, 39, 1090-1102.	1.5	14
2	Formation of dimers of light noble atoms under encapsulation within fullereneâ€™s voids. Nanoscale Research Letters, 2015, 10, 185.	3.1	11
3	<scp>H</scp>e₂@<scp>C</scp>₆₀: Thoughts of the concept of a molecule and of the concept of a bond in quantum chemistry. International Journal of Quantum Chemistry, 2015, 115, 859-867.	1.0	7
4	Density functional theory: Foundations reviewed. Physics Reports, 2014, 544, 123-239.	10.3	91
5	Density Functional Theory and Molecular Interactions: Dispersion Interactions. Structure and Bonding, 2013, , 65-96.	1.0	8
6	On stability and protonation of multielectron systems: The concept of proton affinity. II. Dissociative proton attachment and protonationâ€”Deprotonation mapping. International Journal of Quantum Chemistry, 2012, 112, 382-393.	1.0	0
7	Modeling molecular interactions by analytic potentials: Analytic perturbation treatment. International Journal of Quantum Chemistry, 2012, 112, 2986-2997.	1.0	1
8	I.G. Kaplan: Curriculum vitae. International Journal of Quantum Chemistry, 2012, 112, 2857-2857.	1.0	0
9	Methyl Formate and Its Mono and Difluoro Derivatives: Conformational Manifolds, Basicity, and Interaction with HF Theoretical Investigation. Journal of Physical Chemistry A, 2011, 115, 12586-12601.	1.1	7
10	Stability and protonation of multielectron systems: The concept of proton affinity. I. Vague limits. International Journal of Quantum Chemistry, 2011, 111, 1792-1807.	1.0	7
11	The dimers of glyoxal and acrolein with H2O and HF: Negative intramolecular coupling and blue-shifted Câ€“H stretch. Chemical Physics Letters, 2010, 489, 39-43.	1.2	18
12	Three computational miseâ€enâ€scÃ¨nes of redâ€•and blueâ€shifted hydrogen bonding motifs: Concept of negative intramolecular couplingâ€”What else?. International Journal of Quantum Chemistry, 2010, 110, 104-119.	1.0	12
13	On the Intramolecular Origin of the Blue Shift of Aâ‹¯H Stretching Frequencies: Triatomic Hydrides HAX. Journal of Physical Chemistry A, 2009, 113, 5217-5223.	1.1	33
14	Gold in Hydrogen Bonding Motifâ€”Fragments of Essay. NATO Science for Peace and Security Series A: Chemistry and Biology, 2009, , 315-334.	0.5	0
15	Interaction of uranyl ion with few molecules of water: thought (computational) scenarios with hydrogen bonding motif. Theoretical Chemistry Accounts, 2008, 120, 421-428.	0.5	13
16	The force field picture of molecular shape response. International Journal of Quantum Chemistry, 2008, 108, 1930-1938.	1.0	8
17	Where gold meets a hydrogen bond?. Journal of Molecular Structure, 2008, 880, 23-30.	1.8	46
18	Bonding Rearrangements of Hydrogen-Bonded Complexes Involving Alkynes. Journal of Physical Chemistry A, 2008, 112, 1940-1945.	1.1	8

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19	Blue-Shifted Aâ˜H Stretching Modes and Cooperative Hydrogen Bonding. 1. Complexes of Substituted Formaldehyde with Cyclic Hydrogen Fluoride and Water Clusters. Journal of Physical Chemistry A, 2007, 111, 8177-8187.	1.1	47
20	The Concept of Molecular Shape Response Quantified within Force Field Approach. AIP Conference Proceedings, 2007, , .	0.3	0
21	On the paradigm. Journal of Molecular Structure, 2007, 844-845, 193-199.	1.8	8
22	Formula that accounts a number of atoms within a period of the periodic table. International Journal of Quantum Chemistry, 2007, 107, 372-373.	1.0	2
23	Dicationic states of benzene dimer: Benzene dimer cation and benzene dication parenthood patterns. International Journal of Quantum Chemistry, 2007, 107, 2741-2755.	1.0	7
24	A review on goldâ€“ammonia bonding patterns. Progress in Theoretical Chemistry and Physics, 2007, , 161-191.	0.2	3
25	Neutral Blue-Shifting and Blue-Shifted Hydrogen Bonds. , 2006, , 293-336.		11
26	On the proof by reductio ad absurdum of the Hohenbergâ€“Kohn theorem for ensembles of fractionally occupied states of Coulomb systems. International Journal of Quantum Chemistry, 2006, 106, 1795-1798.	1.0	9
27	On blue shifts of Câ€“H stretching modes of dimethyl ether in hydrogen- and halogen-bonded complexes. Chemical Physics Letters, 2006, 431, 428-433.	1.2	58
28	Theoretical force-field model for blue-shifted hydrogen bonds with fluoromethanes. Chemical Physics, 2006, 329, 313-328.	0.9	37
29	Blue-shifted hydrogen-bonded complexes. II. CH3Fâ‹¯(HF)1â©½nâ©½3 and CH2F2â‹¯(HF)1â©½nâ©½3. Chemical Physics, 2005, 3 77-84.	0.9	51
30	On the original proof by reductio ad absurdum of the Hohenberg-Kohn theorem for many-electron Coulomb systems. International Journal of Quantum Chemistry, 2005, 103, 818-823.	1.0	15
31	The Fate of Dicationic States in Molecular Clusters of Benzene and Related Compounds. Journal of the American Chemical Society, 2005, 127, 16824-16834.	6.6	17
32	Strongly Blue-Shifted Câ˜H Stretches:Â Interaction of Formaldehyde with Hydrogen Fluoride Clusters. Journal of Physical Chemistry A, 2005, 109, 8930-8937.	1.1	58
33	Theoretical study of hydrogenation of thiouracils and their base pairs with adenine. International Journal of Quantum Chemistry, 2004, 99, 841-853.	1.0	8
34	Quantum chemical study of the hydrogen-bonded patterns in A Â· T base pair of DNA: Origins of tautomeric mispairs, base flipping, and Watson-Crick â‡' Hoogsteen conversion. International Journal of Quantum Chemistry, 2003, 91, 695-710.	1.0	55
35	Generation of systematic sequences of even-tempered basis sets: Empirical generating formulae. International Journal of Quantum Chemistry, 2003, 93, 112-120.	1.0	12
36	Theoretical Study of the CH4Â·(H2O)2and CH4. H5O2+Complexes. Three-Hydrogen-Atoms Interaction. Journal of Physical Chemistry A, 2003, 107, 7546-7551.	1.1	22

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37	Blue-Shifted Hydrogen-Bonded Complexes CF3Hâ˜(HF)1â‰nâ‰3. Journal of Physical Chemistry A, 2003, 107, 9724-9729.	1.1	69
38	Theoretical Study of Alkali Metal Pyrrolides in Comparison with nHâ˜Pyrrole. Journal of Physical Chemistry A, 2003, 107, 5427-5438.	1.1	15
39	Theoretical Study of the CHÂ·Â·Â·X-Interaction of Fluoromethanes and Chloromethanes with Fluoride, Chloride, and Hydroxide Anions. Journal of Physical Chemistry A, 2002, 106, 6832-6838.	1.1	62
40	Multiprotonation of Benzene:Â A Theoretical Study. Journal of Physical Chemistry A, 2002, 106, 510-519.	1.1	19
41	Unnatural Covalent DNA Base Pairing:â€‰ Quantum Chemical Study. Journal of Physical Chemistry A, 2002, 106, 9319-9324.	1.1	17
42	Hydrogen Bonding between Phenol and Acetonitrile. Journal of Physical Chemistry A, 2002, 106, 4267-4271.	1.1	58
43	Key properties of monohalogen substituted phenols: interpretation in terms of the electron localization function. Molecular Physics, 2002, 100, 1659-1675.	0.8	29
44	Comments on "Some fundamental problem with zero flux partitioning of electron densities". Theoretical Chemistry Accounts, 2002, 107, 375-377.	0.5	15
45	The origin of spontaneous point mutations in DNA via LÃ¶wdin mechanism of proton tunneling in DNA base pairs: Cure with covalent base pairing*. International Journal of Quantum Chemistry, 2002, 90, 910-923.	1.0	41
46	Mechanism of the oxidation reaction of Cu with N2O via nonadiabatic electron transfer. International Journal of Quantum Chemistry, 2002, 89, 329-340.	1.0	13
47	Existence of strictly diabatic basis sets for the two-state problem. International Journal of Quantum Chemistry, 2002, 89, 255-259.	1.0	37
48	Theoretical Study of Tautomeric Forms of Uracil. 1. Relative Order of Stabilities and Their Relation to Proton Affinities and Deprotonation Enthalpies. Journal of Physical Chemistry A, 2001, 105, 1288-1295.	1.1	111
49	Theoretical Study of Uracil Tautomers. 2. Interaction with Water. Journal of Physical Chemistry A, 2001, 105, 1934-1943.	1.1	100
50	Another look at the electron attachment to nitrous oxide. Journal of Chemical Physics, 2001, 114, 7911-7917.	1.2	35
51	Low Energy Barrier Proton Transfer in Protonated Benzeneâ˜Water Complex. Journal of Physical Chemistry A, 2001, 105, 153-155.	1.1	45
52	Theoretical Study of the CHÂ·Â·Â·O Interaction in FluoromethanesÂ·H2O and ChloromethanesÂ·H2O Complexes. Journal of Physical Chemistry A, 2001, 105, 7118-7125.	1.1	123
53	Modeling Chemisorption of Benzene and Its Hydrogenation on Platinum Surfaces. 1. Complexes of Benzene with Pt and Pt2. Journal of Physical Chemistry B, 2001, 105, 3557-3566.	1.2	15
54	Thiouracils:Â Acidity, Basicity, and Interaction with Water. Journal of Physical Chemistry A, 2001, 105, 3379-3387.	1.1	39

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55	Density functional calculations on protonated and deprotonated thiouracils and their complexes with water. Chemical Physics, 2001, 264, 21-35.	0.9	14
56	Preopening of the DNA base pairs. International Journal of Quantum Chemistry, 2001, 82, 193-204.	1.0	25
57	Thiouracils: Structures, tautomerism, interaction with water, and functioning in RNA and modified DNA base Pairs. Advances in Quantum Chemistry, 2001, 40, 79-102.	0.4	11
58	Hydrogen bonding in benzonitrileâ€“water complexes. Journal of Chemical Physics, 2001, 115, 833-841.	1.2	35
59	Explicit expression for the leaky aquifer function. International Journal of Quantum Chemistry, 2000, 78, 303-305.	1.0	8
60	Ab initio study of L-orientational defect in the hydrogen-bonded pattern of liquid water. Journal of Molecular Structure, 1997, 416, 43-61.	1.8	2
61	Retrospective outlook on computational aspects of energy density functional theory: Explicit and implicit contributions of Enrico Clementi. International Journal of Quantum Chemistry, 1992, 42, 591-626.	1.0	16
62	The Concept of Soliton-Carrier Collective Variable for Proton Transfer in Extended Hydrogen-Bonded Systems: Overview. NATO ASI Series Series B: Physics, 1992, , 105-119.	0.2	1
63	Study of tunnelling in symmetrical double-Morse hydrogen bonds via the instanton-soliton approach: large polarizability and isotopic effect. Computational and Theoretical Chemistry, 1991, 235, 157-183.	1.5	9
64	Quantum rigid dipole in a permanent electric field. I. Rigorous treatment. International Journal of Quantum Chemistry, 1991, 40, 33-53.	1.0	9
65	Quantum rigid dipole in a permanent electric field. II. Model of librational motion in liquid water and ice Ih: Preliminary results. International Journal of Quantum Chemistry, 1991, 40, 55-66.	1.0	1
66	Collective proton transfer in the (Aî—¸Hâ€¦)âˆž system with double-Morse symmetric potential. I. Model of proton kink defect. Chemical Physics, 1990, 143, 359-370.	0.9	30
67	Energy Density Functional Theory of Many-Electron Systems. , 1990, , .		305
68	The cooperative model for orientational defects in ice: Continuum approach. Chemical Physics Letters, 1987, 141, 346-349.	1.2	15
69	On the red shift of OH stretching region vibrations in ice and water. International Journal of Quantum Chemistry, 1986, 30, 495-508.	1.0	6
70	Algebraic structure of fermion density matrices. II. International Journal of Quantum Chemistry, 1981, 19, 505-514.	1.0	2
71	Reduced-density-matrix theory and algebraic structures. International Journal of Quantum Chemistry, 1978, 13, 719-730.	1.0	2
72	General and Theoretical Aspects of Phenols. , 0, , 1-198.		16