Mohammad Solimannejad

List of Publications by Year
in descending order

100	1,682	304743	361022
papers	citations	22 h-index	35 g-index

102	102	102	890
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	A computational DFT insight into adsorption properties of urea and creatinine molecules on pristine B24O24 nanocluster. Structural Chemistry, 2023, 34, 577-584.	2.0	3
2	Empowering hydrogen storage performance of B4C3Âmonolayer through decoration with lithium: A DFT study. Surfaces and Interfaces, 2022, 29, 101723.	3.0	15
3	B3O3 monolayer with dual application in sensing of COVID-19 biomarkers and drug delivery for treatment purposes: A periodic DFT study. Journal of Molecular Liquids, 2022, 354, 118855.	4.9	19
4	Potential application of XC₃ (Xâ€‰=â€‰B, N) nanosheets in drug delivery of hydroxyurea anticancer drug: a comparative DFT study. Molecular Physics, 2022, 120, .	1.7	19
5	Systematic study of cooperative interplay between single-electron pnicogen bond and halogen bond in X₃CÂ·Â·Â·PH₂YÂ·Â·Â·ClY (X=H, CH₃; Y=CN, NC) complexes in two different minima configuration. Molecular Physics, 2022, 120, .	1.7	1
6	The Porous B6N6 Boron Nitride Covalent Organic Framework as a Potential Platform for Sensing and Delivering Lomustine Anticancer Drug: A First-Principles Study. Journal of Inorganic and Organometallic Polymers and Materials, 2022, 32, 4216-4222.	3.7	6
7	Liâ€decorated <scp>Al₂C</scp> monolayer as a potential template for hydrogen storage: A firstâ€principles perspective. International Journal of Quantum Chemistry, 2021, 121, e26528.	2.0	22
8	Toxic volatile organic compounds sensing by Al2C monolayer: A first-principles outlook. Journal of Hazardous Materials, 2021, 403, 123600.	12.4	22
9	Hydrogen storage on pristine and Li-decorated BC₆N monolayer from first-principles insights. Molecular Physics, 2021, 119, e1827177.	1.7	24
10	First-principles survey on the pristine BC2N monolayer as a promising vehicle for delivery of Î²-lapachone anticancer drug. Journal of Molecular Liquids, 2021, 321, 114917.	4.9	22
11	Periodic DFT insights into hydrogen storage of a B₄CN₃ nanosheet. New Journal of Chemistry, 2021, 45, 2463-2469.	2.8	22
12	B₃O₃ monolayer: an emerging 2D material for CO₂ capture. New Journal of Chemistry, 2021, 45, 15328-15335.	2.8	20
13	Adsorption of chloroquine and hydroxychloroquine as potential drugs for SARS-CoV-2 infection on BC₃ nanosheets: a DFT study. New Journal of Chemistry, 2021, 45, 17976-17983.	2.8	16
14	Gas-sensing performance of BC₃ nanotubes for detecting poisonous cyanogen gas: a periodic DFT approach. New Journal of Chemistry, 2021, 45, 11574-11584.	2.8	14
15	Pristine B3CN4 monolayer for hydrogen storage: A first-principles approach. Physics Letters, Section A: General, Atomic and Solid State Physics, 2021, 391, 127116.	2.1	20
16	High-Performance Hydrogen Storage Properties of Li-Decorated B₂N₂ Nanosheets: A Periodic Density Functional Theory Study. Energy & Fuels, 2021, 35, 6858-6867.	5.1	33
17	Titanium-benzene complex as a molecular oxide adsorbent: a first principles approach. Journal of Molecular Modeling, 2021, 27, 242.	1.8	2
18	Sensing ability of 2D Al2C monolayer toward toxic pnictogen hydrides: A first-principles perspective. Sensors and Actuators A: Physical, 2021, 331, 113000.	4.1	10

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19	H2 storage and equilibrium isotope effect for Be, Li, and Ti-doped closoborate complexes. Structural Chemistry, 2021, 32, 1489-1504.	2.0	1
20	First-principles studies on two-dimensional B3O3 adsorbent as a potential drug delivery platform for TEPA anticancer drug. Journal of Molecular Modeling, 2021, 27, 347.	1.8	16
21	Hydrazine trapping ability of Si12C12 fullerene-like nanoclusters: a DFT study. Structural Chemistry, 2020, 31, 133-140.	2.0	6
22	Hydrogen abstraction of methanimine by X12N12 (X = B, Al) nanoclusters: a DFT study. Structural Chemistry, 2020, 31, 447-454.	2.0	0
23	First-principles study of superior hydrogen storage performance of Li-decorated Be2N6 monolayer. International Journal of Hydrogen Energy, 2020, 45, 19465-19478.	7.1	24
24	BC3 graphene-like monolayer as a drug delivery system for nitrosourea anticancer drug: A first-principles perception. Applied Surface Science, 2020, 525, 146577.	6.1	44
25	The potential application of borazine (B3N3)-doped nanographene decorated with halides as anode materials for Li-ion batteries: a first-principles study. Journal of Molecular Modeling, 2020, 26, 157.	1.8	11
26	Ab initio calculations and molecular dynamics simulation of H2 adsorption on CN3Be3+ cluster. Structural Chemistry, 2020, 31, 1757-1763.	2.0	2
27	Functionalization of BC3 nanotubes with substituted pyridine: a DFT study. Materials Research Express, 2019, 6, 065016.	1.6	2
28	Tuning the electronicâ€optical properties of porphyrinâ€like porous C₂₄N₂₄ fullerene with (Li₃O)_{nÂ=Â(1â€“5)} decoration. A computational study. Applied Organometallic Chemistry, 2019, 33, e4654.	3.5	9
29	Electronic properties of B12N12 fullereneâ€“like nanoclusters functionalized with Schiff bases: a DFT study. Structural Chemistry, 2019, 30, 979-987.	2.0	2
30	Adsorption of rare gases on the C₂₀nanocage: a theoretical investigation. Materials Research Express, 2018, 5, 035006.	1.6	12
31	Correlating cluster size and NLO response of complexes aggregated with bifurcated metal bonds: a DFT study. Structural Chemistry, 2018, 29, 119-127.	2.0	1
32	The effect of the hydrogen fluoride chain on the aromaticity of C6H6 in the C6H6Â·Â·Â·(HF)1â€“4 complexes. Molecular Physics, 2018, 116, 313-322.	1.7	1
33	A novel receptor for detection of Zn2+ metal ion and Fâ^', H2PO4 â^' and AcOâ^' anions in aqueous media: a DFT study. Chemical Papers, 2018, 72, 719-729.	2.2	13
34	Silicon carbide nanotubes (SiCNTs) serving for catalytic decomposition of toxic diazomethane (DAZM) gas: a DFT study. Molecular Physics, 2018, 116, 414-422.	1.7	3
35	Can bowl-like B30 nanostructure sense toxic cyanogen gas in air?: a theoretical study. Molecular Physics, 2018, 116, 2196-2204.	1.7	5
36	A computational study of interplay between hydride bonding and cationâ€“Ï€ interactions: H-Mg-HÂ·Â·Â·XÂ·Â·Â·Y triads (X = Li+, Na+, Y = C2H2, C2H4, C6H6) as model systems. Molecular Physics, 2017, 115, 825-830.	1.7	4

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37	Evaluation of one-dimensional potential energy surfaces for prediction of spectroscopic properties of hydrogen bonds in linear bonded complexes. Journal of Molecular Modeling, 2017, 23, 157.	1.8	3
38	Sensing performance of Cu-decorated Si₁₂C₁₂ nanocage towards toxic cyanogen gas: a DFT study. Materials Research Express, 2017, 4, 045011.	1.6	7
39	Nonlinear Optical (NLO) Response of Si12C12 Nanocage Decorated with Alkali Metals (Mâ€‰=â€‰Li, Na and K): A Theoretical Study. Journal of Inorganic and Organometallic Polymers and Materials, 2017, 27, 1234-1242.	3.7	16
40	Li n @B36 (nÂ=Â1, 2) Nanosheet with Remarkable Electro-Optical Properties: A DFT Study. Journal of Electronic Materials, 2017, 46, 4420-4425.	2.2	14
41	Boron nitride nanotube (BNNT) as a sensor of hydroperoxyl radical (HO2): A DFT study. Journal of the Iranian Chemical Society, 2017, 14, 471-476.	2.2	32
42	Selective detection of toxic cyanogen gas in the presence of O 2 , and H 2 O molecules using a AlN nanocluster. Physics Letters, Section A: General, Atomic and Solid State Physics, 2016, 380, 2854-2860.	2.1	12
43	Microsolvation of CH+ in helium: An ab initio study. Journal of Theoretical and Computational Chemistry, 2016, 15, 1650018.	1.8	1
44	Symmetric bifurcated halogen bonds: substituent and cooperative effects. Molecular Physics, 2016, 114, 3610-3619.	1.7	4
45	Nonlinear Optical (NLO) Response of Pristine and Functionalized Dodecadehydrotribenzo[18]annulene ([18]DBA): A Theoretical Study. Bulletin of the Chemical Society of Japan, 2016, 89, 692-699.	3.2	25
46	Mild and green synthesis of tetrahydrobenzopyran, pyranopyrimidinone and polyhydroquinoline derivatives and DFT study on product structures. Research on Chemical Intermediates, 2016, 42, 1165-1179.	2.7	63
47	Mutual influence between anionâ€“Ï€ and pnicogen bond interactions: The enhancement of Pâ‹¯N and Pâ‹¯O interactions by an anionâ€“Ï€ bond. Journal of Molecular Graphics and Modelling, 2015, 57, 99-105.	2.4	22
48	Ab initiointermolecular potential energy surface of NeÂ·Â·Â·NCCN van der Waals complex: effect of the place of midbond function on the interaction. Molecular Physics, 2015, 113, 3303-3311.	1.7	5
49	Effect of cooperativity in lithium bonding on the strength of halogen bonding and tetrel bonding: (LiCN)nÂ·Â·Â·ClYF3 and (LiCN)nÂ·Â·Â·YF3Cl (Y= C, Si and nâ€‰=â€‰1â€“5) complexes as a working model. Journal of Molecular Modeling, 2015, 21, 183.	1.8	29
50	Rovibrational energy and spectroscopic constant calculations of complexes pairing via dihydrogen bonds. Journal of Molecular Modeling, 2015, 21, 119.	1.8	1
51	Tuning of chalcogen bonds by cationâ€“Ï€ interactions: cooperative and diminutive effects. Journal of Molecular Modeling, 2015, 21, 300.	1.8	8
52	Effect of cooperativity in lithium bonding on the strength of hydrogen bonding: (LiCN) n Â·Â·Â·HX (nÂ=Â1â€“5,) Tj ETQq0 0 0 rgBT /Over	2.0	4
53	Ab initiointermolecular potential energy surfaces for the Arâ€“NCCN van der Waals complexes. Molecular Physics, 2014, 112, 2924-2932.	1.7	9
54	A Computational Study of 1â€²:â€²1 and 1â€²:â€²2 Complexes of Naphthalene with Dimethyl Ether. Zeitschrift Fur Physikalische Chemie, 2014, 228, 115-125.	2.8	0

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55	A theoretical evidence for mutual influence between SÂ·Â·Â·N(C) and hydrogen/lithium/halogen bonds: competition and interplay between Ï€-hole and Ïƒ-hole interactions. Structural Chemistry, 2014, 25, 1197-1205.	2.0	51
56	Mutual influence between conventional and unconventional lithium bonds. Journal of Molecular Graphics and Modelling, 2014, 49, 129-137.	2.4	7
57	Cooperative interaction between Ï€-hole and single-electronÏƒ-hole interactions in O2SÂ·Â·Â·NCXÂ·Â·Â·CH3and O2SeÂ·Â·Â·NCXÂ·Â·Â·CH3complexes (X = F, Cl, Br and I). Molecular Physics, 2014, 112, 2078-2084.	1.7	20
58	Cooperative and diminutive interplay between the sodium bonding with hydrogen and dihydrogen bondings in ternary complexes of NaC₃N with HMgH and HCN (HNC). Molecular Physics, 2014, 112, 2017-2022.	1.7	18
59	Enhancement effect of lithium bonding on the strength of pnicogen bonds: XH₂PÂ·Â·Â·NCLiÂ·Â·Â·NCY as a working model (X = F, Cl; Y = H, F, Cl, CN). Molecular Physics, 2014, 112, 2058-2062.	1.7	24
60	Interplay and competition between the lithium bonding and halogen bonding: R₃CÂ·Â·Â·XCNÂ·Â·Â·LiCN and R₃CÂ·Â·Â·LiCNÂ·Â·Â·XCN as a working model (R = H,) Tj ETQq1 0 0 rgBT /Overloc	2.0	32
61	Substituent effects on cooperativity between lithium bonds. International Journal of Quantum Chemistry, 2014, 114, 295-301.	2.0	16
62	Hydrogen bond strengthening of cisâ€“trans glyoxal dimers in electronic excited states: A theoretical study. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2014, 122, 337-342.	3.9	5
63	Revealing substituent effects on the concerted interaction of pnicogen, chalcogen, and halogen bonds in substituted s-triazine ring. Structural Chemistry, 2013, 24, 1705-1711.	2.0	18
64	Ab initio study of ternary radicalâ€“molecule complexes between HCN(HNC) and HO(HS) species. Structural Chemistry, 2013, 24, 1493-1498.	2.0	10
65	A computational study of 1:1 and 1:2 complexes of nitryl halides (O2NX) with HCN and HNC. Structural Chemistry, 2013, 24, 651-659.	2.0	20
66	Ab initio study of water clustering in the presence of a methyl radical. Structural Chemistry, 2013, 24, 491-497.	2.0	3
67	Substituent Effects on the Cooperativity of Halogen Bonding. Journal of Physical Chemistry A, 2013, 117, 5551-5557.	2.5	73
68	Analysis of torsional barrier height of HSNO as the simplest S-nitrosothiol. Journal of Chemical Sciences, 2013, 125, 913-917.	1.5	3
69	A Novel Metal Organic Compound of Al(III): Synthesis, Crystal Structure, Spectroscopic and Theoretical Study. Journal of Chemical Crystallography, 2012, 42, 1152-1161.	1.1	3
70	Investigation of the formation of acid rain based on the sulfur tetroxide (SO4 (C2v)) and OH radical reaction. Structural Chemistry, 2012, 23, 1609-1615.	2.0	6
71	Competition and Interplay between Ïƒ-Hole and Ï€-Hole Interactions: A Computational Study of 1:1 and 1:2 Complexes of Nitryl Halides (O₂NX) with Ammonia. Journal of Physical Chemistry A, 2012, 116, 5199-5206.	2.5	86
72	Cooperative and Diminutive Interplay Between Lithium and Dihydrogen Bonding in F₃YLiâ€¦NCHâ€¦HMH and F₃YLiâ€¦HMHâ€¦HCN Triads (Y=C, Si; M=Be, Mg). ChemPhysChem, 2012, 13, 3158-3162.	2.1	20

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73	A theoretical study of 1:1 and 1:2 complexes of acetylene with nitrosyl hydride. Structural Chemistry, 2012, 23, 847-856.	2.0	7
74	Theoretical study of molecular interactions of phosphorus ylide with HF, HCN, and HN3. Structural Chemistry, 2012, 23, 1155-1161.	2.0	5
75	Computational study on the reaction mechanism of the gas-phase atom-negative ion of SÂ+ÂNO2 â˜': comparative study of mechanism with SÂ+ÂO3 reaction as isoelectronic and isostructure systems. Structural Chemistry, 2012, 23, 381-392.	2.0	5
76	Cooperativity between the hydrogen bonding and halogen bonding in F₃CXâ€‰Â·Â·Â·â€‰NCH(CNH)â€‰Â·Â·Â·â€‰NCH(CNH) complexes (X=Cl, Br). Molecular Physics, 2011, 109, 1641-1648	1.7	45
77	SHÂ·Â·Â·N and SHÂ·Â·Â·P blue-shifting H-bonds and NÂ·Â·Â·P interactions in complexes pairing HSN with amines and phosphines. Journal of Chemical Physics, 2011, 134, 024312.	3.0	126
78	Hydrogen-bonded clusters of hydroperoxyl radical with ammonia: a theoretical study. Structural Chemistry, 2011, 22, 193-199.	2.0	2
79	HNO(H2O) n (nÂ=Â1â€“4) clusters: a theoretical study. Structural Chemistry, 2011, 22, 865-871.	2.0	8
80	Unconventional Hâ€bonds: SHÂ·Â·Â·N interaction. International Journal of Quantum Chemistry, 2011, 111, 3196-3200.	2.0	17
81	Glyoxal oligomers: A computational study. International Journal of Quantum Chemistry, 2011, 111, 3057-3069.	2.0	9
82	Stabilities and properties of ozoneâ€“sulphuryl fluoride (O₃â€“SO₂F₂) complexes:a computational study. Molecular Simulation, 2011, 37, 1071-1076.	2.0	1
83	Cooperative and Diminutive Unusual Weak Bonding In F₃CXÂ·Â·Â·HMgHÂ·Â·Â·Y and F₃CXÂ·Â·Â·YÂ·Â·Â·HMgH Trimers (X = Cl, Br; Y = HCN, and HNC). Journal of Physical Chemistry A, 2010, 114, 12106-12111.	2.5	80
84	A Computational Study of the Potential Energy Surface of Peroxyformic Acid Dimers. Journal of Physical Chemistry A, 2010, 114, 9388-9393.	2.5	5
85	Theoretical study and atoms in molecule analysis of hydrogen bonded clusters of ammonia and isocyanic acid. Structural Chemistry, 2009, 20, 1087-1092.	2.0	19
86	Nature of interactions in open-shell complexes pairing H₂X with HXX, X=S,O. Molecular Physics, 2009, 107, 713-719.	1.7	14
87	Inverse hydrogen bonds between XeH2 and hydride and fluoride derivatives of Li, Be, Na and Mg. Theoretical Chemistry Accounts, 2008, 121, 181-186.	1.4	13
88	Complexes Pairing Hypohalous Acids with Nitrosyl Hydride. Blue Shift of a NH Bond That Is Uninvolved in a H-Bond. Journal of Physical Chemistry A, 2008, 112, 4120-4124.	2.5	41
89	Weakly Bound Complexes of N2O:â€‰ An ab Initio Theoretical Analysis Toward the Design of N2O Receptors. Journal of Physical Chemistry A, 2007, 111, 2077-2083.	2.5	10
90	Analysis of Complexes Pairing Hydroperoxyl Radical with Peroxyformic Acid. Journal of Physical Chemistry A, 2007, 111, 10717-10721.	2.5	15

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91	Theoretical Evidence for a NHÂ·Â·Â·XC Blue-Shifting Hydrogen Bond:â€‰ Complexes Pairing Monohalomethanes with HNO. Journal of Physical Chemistry A, 2007, 111, 4431-4435.	2.5	33
92	Stabilities and Properties of Complexes Pairing Hydroperoxyl Radical with Monohalomethanes. Journal of Physical Chemistry A, 2006, 110, 5948-5951.	2.5	24
93	Competition between Nonclassical Hydrogen-Bonded Acceptor Sites in Complexes of Neutral AH2Radicals (A = B, Al, and Ga):Â A Theoretical Investigation. Journal of Physical Chemistry A, 2006, 110, 10817-10821.	2.5	26
94	Nonperturbative solutions for one-dimensional SchrÃ¶dinger equation with position-dependent mass. International Journal of Quantum Chemistry, 2006, 106, 1027-1031.	2.0	6
95	Theoretical study of structure, stability and infrared spectra of CH3Xî—¸SO3 (X = F, Cl, Br) complexes. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2005, 61, 373-375.	3.9	2
96	Computational Investigation of the Weakly Bound Dimers HOXÂ·Â·Â·SO3(X = F, Cl, Br). Journal of Physical Chemistry A, 2005, 109, 825-831.	2.5	28
97	Reply to Comment on â€œComputational Investigation of SO3â^'NH3-nXn(n= 0â^'3; X = F, Cl) Interactionsâ€. Journal of Physical Chemistry A, 2005, 109, 2412-2412.	2.5	0
98	Theoretical Investigation of the Dihydrogen Bond Linking MH2 with HCCRgF (M = Zn, Cd; Rg = Ar, Kr). Journal of Physical Chemistry A, 2005, 109, 11933-11935.	2.5	32
99	Computational Investigation of SO3â^'NH3-nXn(n= 0â^'3; X = F, Cl) Interactions. Journal of Physical Chemistry A, 2004, 108, 10342-10345.	2.5	9
100	G2 Molecular Orbital Investigation of OCH+â^'XH, OCH+â^'X2, and OCH+â^'XY(YX) (X = Y = F, Cl, and Br) Proton Bond Complexes. Journal of Physical Chemistry A, 2004, 108, 4769-4772.	2.5	4