Fu-de Ren

List of Publications by Year
in descending order

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60	612	623574	713332
papers	citations	14 h-index	21 g-index

62	62	62	358
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	A theoretical investigation into the cooperativity effect on the TNT melting point under external electric field. Journal of Molecular Modeling, 2021, 27, 4.	0.8	4
2	Theoretical prediction of the trigger linkage, cage strain, and explosive sensitivity of CL-20 in the external electric fields. Journal of Molecular Modeling, 2021, 27, 85.	0.8	7
3	Theoretical investigation into the solvent effect on the thermal decomposition of RDX in tetrahydrofuran, acetone, toluene, and benzene. Journal of Molecular Modeling, 2021, 27, 343.	0.8	1
4	A correction into â€œTheoretical prediction of the trigger linkage, cage strain and explosive sensitivity of CL-20 in the external electric fieldsâ€• Journal of Molecular Modeling, 2021, 27, 352.	0.8	0
5	Theoretical evaluation to improve the performance of composite wax powder: cooperativity effects involving the strong Na⁺Â·Â·Â·Ï€/Ïƒ and weak hydrogen-bonding interactions in the complex of graphene oxide with Na⁺ and CH₄. Molecular Physics, 2020, 118, e1612106.	0.8	3
6	Theoretical explanation for the DNA cleavage by GO with cation: anti-cooperativity effect among the Ï€â‹¯Ï€, cationâ‹¯Ï€/Ïƒ and H-bonding interactions in cytosineâ‹¯GOâ‹¯Mⁿ⁺ (Mⁿ⁺â€‰=â€‰Na⁺, Mg²⁺, Al³⁺). Molecular Physics, 2020, 118, e1692149.	0.8	2
7	External electric field reduces the explosive sensitivity: a theoretical investigation into the hydrogen transference kinetics of the NH2NO2â˚™â˚™â˚™H2O complex. Journal of Molecular Modeling, 2020, 26, 351.	0.8	7
8	Theoretical prediction of the impact sensitivities of energetic C-nitro compounds. Journal of Molecular Modeling, 2020, 26, 219.	0.8	4
9	Hydration and swelling: a theoretical investigation on the cooperativity effect of H-bonding interactions between p-hydroxy hydroxymethyl calix[4]/[5]arene and H2O by many-body interaction and density functional reactivity theory. Journal of Molecular Modeling, 2020, 26, 190.	0.8	2
10	Theoretical investigation into the cooperativity effect of 1,4-dimethoxy-d-glucosamine complex with Na+ and H2O. Journal of Molecular Modeling, 2020, 26, 203.	0.8	1
11	A dynamic and electrostatic potential prediction of the prototropic tautomerism between imidazole 3-oxide and 1-hydroxyimidazole in external electric field. Journal of Molecular Modeling, 2019, 25, 330.	0.8	6
12	Cooperativity effect of the Ï€â‹¯Ï€ interaction between drug and DNA on intercalative binding induced by H-bonds: a QM/QTAIM investigation of the curcuminâ‹¯adenineâ‹¯H₂O model system. Physical Chemistry Chemical Physics, 2019, 21, 11871-11882.	1.3	3
13	Theoretical prediction of the trigger linkages, surface electrostatic potentials, and explosive sensitivities of 1,4-dinitroimidazole-N-oxide in the external electric fields. Journal of Molecular Modeling, 2019, 25, 368.	0.8	1
14	Theoretical and experimental investigation into a eutectic system of 3,4-dinitropyrazole and 1-methyl-3,4,5-trinitropyrazole. Journal of Molecular Modeling, 2018, 24, 9.	0.8	12
15	Theoretical investigation into the cooperativity effect between the intermolecular Ï€â˚™Ï€ and H-bonding interactions in the curcuminâ˚™cytosineâ˚™H2O system. Journal of Molecular Modeling, 2018, 24, 298.	0.8	3
16	Theoretical investigation into the influence of molar ratio on binding energy, mechanical property and detonation performance of 1,3,5,7-tetranitro-1,3,5,7-tetrazacyclo octane (HMX)/1-methyl-4,5-dinitroimidazole (MDNI) cocrystal explosive. Computational and Theoretical Chemistry, 2017, 1109, 27-35.	1.1	10
17	Theoretical insight into the BH3Â·HCN adsorption on the Co(100) and Co(110) surfaces as hydrogen storage. Journal of Molecular Modeling, 2017, 23, 126.	0.8	10
18	A dynamic prediction of stability for nitromethane in external electric field. RSC Advances, 2017, 7, 47063-47072.	1.7	22

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19	Theoretical investigation of the effects of the molar ratio and solvent on the formation of the pyrazoleâ€“nitroamine cocrystal explosive 3,4-dinitropyrazole (DNP)/2,4,6,8,10,12-hexanitrohexaazaisowurtzitane (CL-20). Journal of Molecular Modeling, 2017, 23, 353.	0.8	13
20	Growth morphology of CL-20/HMX cocrystal explosive: insights from solvent behavior under different temperatures. Journal of Molecular Modeling, 2017, 23, 360.	0.8	25
21	Theoretical investigation of the safety of nitroguanidine-based PBXs containing the nonpolar desensitizing agent polytetrafluoroethylene. Journal of Molecular Modeling, 2017, 23, 346.	0.8	3
22	Molecular dynamics simulation and density functional theory insight into the cocrystal explosive of hexaazaisowurtzitane/nitroguanidine. International Journal of Quantum Chemistry, 2016, 116, 88-96.	1.0	21
23	A dynamics prediction of nitromethane â†' methyl nitrite isomerization in external electric field. Journal of Molecular Modeling, 2016, 22, 96.	0.8	19
24	A theoretical prediction of the relationships between the impact sensitivity and electrostatic potential in strained cyclic explosive and application to H-bonded complex of nitrocyclohydrocarbon. Journal of Molecular Modeling, 2016, 22, 97.	0.8	9
25	Theoretical insight into the sensitive mechanism of multilayer-shaped cocrystal explosives: compression and slide. Journal of Molecular Modeling, 2016, 22, 108.	0.8	2
26	Theoretical insight into the binding energy and detonation performance of Îµ-, Î³-, Î²-CL-20 cocrystals with Î²-HMX, FOX-7, and DMF in different molar ratios, as well as electrostatic potential. Journal of Molecular Modeling, 2016, 22, 123.	0.8	35
27	Theoretical insights into the stabilities, detonation performance, and electrostatic potentials of cocrystals containing Îµ- or Î²-HMX and TATB, FOX-7, NTO, or DMF in various molar ratios. Journal of Molecular Modeling, 2016, 22, 249.	0.8	10
28	Theoretical Insight into the Influences of Molecular Ratios on Stabilities and Mechanical Properties, Solvent Effect of HMX/FOX-7 Cocrystal Explosive. Journal of Energetic Materials, 2016, 34, 426-439.	1.0	25
29	A theoretical prediction of the possible trigger linkage of CH3NO2 and NH2NO2 in an external electric field. Journal of Molecular Modeling, 2015, 21, 145.	0.8	29
30	Theoretical insight into the co-crystal explosive of 2,4,6,8,10,12-hexanitrohexaazaisowurtzitane (CL-20)/1,1-diamino-2,2-dinitroethylene (FOX-7). Computational Materials Science, 2015, 107, 33-41.	1.4	46
31	A theoretical investigation into the strength of Nâ€“NO2 bonds, ring strain and electrostatic potential upon formation of intermolecular H-bonds between HF and the nitro group in nitrogen heterocyclic rings C n H2n Nâ€“NO2 (nâ€‰=â€‰2â€“5), RDX and HMX. Journal of Molecular Modeling, 2015, 21, 302.	0.8	4
32	A theoretical study on the strength of the Câ€“NO2 bond and ring strain upon the formation of the intermolecular H-bonding interaction between HF and nitro group in nitrocyclopropane, nitrocyclobutane, nitrocyclopentane or nitrocyclohexane. Journal of Molecular Modeling, 2015, 21, 114.	0.8	8
33	Theoretical insights into the structures and mechanical properties of HMX/NQ cocrystal explosives and their complexes, and the influence of molecular ratios on their bonding energies. Journal of Molecular Modeling, 2015, 21, 245.	0.8	27
34	A B3LYP and MP2(full) theoretical investigation into the cooperativity effect between dihydrogen-bonding and Hâ€“Mâˆ™â‹¯Ï€ (Mâ€‰=â€‰Li, Na, K) interactions among HF, MH with the Ï€-electron donor C2H2, C2H4 or C6H6. Journal of Molecular Modeling, 2013, 19, 3153-3163.	0.8	4
35	A comparative theoretical investigation into the strength of the trigger-bond in the Na+, Mg2+ and HF complexes involving the nitro group of Râ€“NO2 (Râ€‰=â€‰â€“CH3, â€“NH2 and â€“OCH3) or the Câ€‰=â€‰C bond of (E)-O2Nâ€“CHâ€‰=â€‰CHâ€“NO2. Journal of Molecular Modeling, 2013, 19, 2499-2507.	0.8	2
36	A B3LYP and MP2(full) theoretical investigation into the strength of the C-NO2 bond upon the formation of the molecule-cation interaction between Na+ and the nitro group of nitrotriazole or its methyl derivatives. Journal of Molecular Modeling, 2013, 19, 453-463.	0.8	5

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37	A B3LYP and MP2(full) theoretical investigation into the strength of the Câ€“NO2 bond upon the formation of the intermolecular hydrogen-bonding interaction between HF and the nitro group of nitrotriazole or its methyl derivatives. Journal of Molecular Modeling, 2013, 19, 511-519.	0.8	11
38	A B3LYP AND MP2(FULL) THEORETICAL INVESTIGATION INTO THE Câ€“NO2 BOND STRENGTH UPON THE FORMATION OF HF OR Na+ COMPLEX INVOLVING THE NITRO GROUP OF NITRO-1,2,4-TRIAZOLE. Journal of Theoretical and Computational Chemistry, 2013, 12, 1350043.	1.8	1
39	A B3LYP and MP2(full) theoretical investigation into explosive sensitivity upon the formation of the moleculeâ€“cation interaction between the nitro group of RNO2 (R=â€“CH3, â€“NH2, â€“OCH3) and Na+, Mg2+ or Al3+. Computational and Theoretical Chemistry, 2012, 991, 107-115.	1.1	3
40	A B3LYP and MP2(full) theoretical investigation into explosive sensitivity upon the formation of the intermolecular hydrogen-bonding interaction between the nitro group of RNO2 (R=â€“CH3, â€“NH2,) Tj ETQq0 0 0 rgBT /Overlock 10 Tf	1.1	11
41	A B3LYP and MP2(full) theoretical investigation on the cooperativity effect between cationâ€“molecule and hydrogen-bonding interactions in the O-cresol complex with Na+. Computational and Theoretical Chemistry, 2012, 996, 91-102.	1.1	11
42	A B3LYP and MP2(full) theoretical investigation into explosive sensitivity upon the formation of the molecule-cation interaction between the nitro group of 3,4-dinitropyrazole and H+, Li+, Na+, Be2+ or Mg2+. Journal of Molecular Modeling, 2012, 18, 2105-2115.	0.8	13
43	A (U)MP2(full) and (U)CCSD(T) theoretical investigation into the substituent effects on the intermolecular T-shaped Fâ€“Hâ€¦Ï€ interactions between HF and LBBL (L = â^'H, â^'CO, :NN, â€“Cl, â€“CN and â€“NC). Journal of Molecular Modeling, 2012, 18, 2959-2969.	1.8	1
44	A MP2(full) and CCSD(T) theoretical investigation on the dihydrogen-bonded interactions between HNa and RBBH (R=F, Cl, H, CN, NC and CO). Computational and Theoretical Chemistry, 2011, 977, 201-208.	1.1	6
45	A (U)MP2(full) and (U)CCSD(T) theoretical investigation into the substituent effects on the cationâ€“Ï€ interactions between M+ (M=Li or Na) and LBBL (L=H, CH3, OH, CN, NC, F, :CO, :NN, :BH, :CNâ^', :NCâ^' and) Tj ETQq1 1 0.784314 rgBT	1.1	4
46	Can the positive aromatic ring be as Ï€-electron donor in Ï€-halogen bond? A MP2 theoretical investigation on the unusual Ï€-halogen bond interaction between three-membered ring $$ left() Tj ETQq0 0 0 rgBT /Overlock 10 Tf 50 3 929-937.	0.8	6
47	A MP2 and CCSD(T) theoretical investigation on the weak dihydrogen-bonded interactions between HBBH (1Î"g) and HM (M=Li, Na, K, BeH, MgH or CaH). Computational and Theoretical Chemistry, 2011, 963, 463-469.	1.1	7
48	A B3LYP and MP2 theoretical investigation into host-guest interaction between calix[4]arene and Li+ or Na+. Journal of Molecular Modeling, 2010, 16, 589-598.	0.8	11
49	A UB3LYP and UMP2 theoretical investigation on unusual cationâ€“Ï€ interaction between the triplet state HB=BH ($$ {}^3Sigma_g^{-} $$) and H+, Li+, Na+, Be2+ or Mg2+. Journal of Molecular Modeling, 2010, 16, 615-627.	0.8	12
50	Theoretical investigation on the structures and thermodynamic properties of mixed boron-, nitrogen- and oxygen-containing three- and four-membered rings B N OH (n= 0â€“3, m= 0â€“3, p= 0â€“3). Computational and Theoretical Chemistry, 2010, 942, 121-130.	1.5	1
51	A (U)MP2(full) and (U)CCSD(T) theoretical investigation on the substituent effect on the cationâ€“Ï€ interactions between Na+ and LCCL (L=H, CH3, OH, F, Cl, CO, NN, CNâ^', NCâ^' and OHâ^'). Computational and Theoretical Chemistry, 2010, 956, 1-9.	1.5	8
52	A MP2(full) theoretical investigation on the Ï€-halogen interaction between OCBBCO and X1X2 (X1,) Tj ETQq0 0 0 rgBT /Overlock 10 Tf	1.5	7
53	A theoretical study on unusual intermolecular T-shaped Xâ€“H...Ï€ interactions between the singlet state HB=BH and HF, HCl, HCN or H2C2. Journal of Molecular Modeling, 2009, 15, 515-523.	0.8	17
54	Can the BB multiple bonds be as the stronger hydrogen-bond proton acceptors than the CC multiple bonds: A comparative theoretical investigation on unusual intermolecular T-shaped XHâ€¦Ï€ interaction between HF and HBBH (), HBBH (1Î"g), OCBBCO, H2CCH2 or HCCH. Computational and Theoretical Chemistry, 2009, 896, 38-43.	1.5	12

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55	Theoretical investigation on geometries and aromaticity of mixed boron-, nitrogen- and furanoxo-containing five-membered rings B2N2OHp (p=0â€“2). Computational and Theoretical Chemistry, 2009, 909, 13-18.	1.5	12
56	A B3LYP and MP2 theoretical investigation on unusual cation-Ï€ interaction between the singlet state HBBH (1Î”g) and H+, Li+, Na+, Be2+ or Mg2+. Computational and Theoretical Chemistry, 2009, 909, 79-85.	1.5	11
57	A MP2(full) and CCSD(T) theoretical investigation on unusual cationâ€“Ï€ interaction between OCBBCO and H+, Li+, Na+, Be2+ or Mg2+. Computational and Theoretical Chemistry, 2009, 913, 221-227.	1.5	14
58	Can BB triple bond be as potential proton acceptor: An ab initio study on unusual intermolecular T-shaped Xâ€“HÂ·Â·Â·Ï€ interactions between OCBBCO and HF, HCl, HCN or H2C2. Chemical Physics Letters, 2008, 455, 32-37.	1.2	19
59	Unusual intermolecular T-shaped Xâ€“Hâ€¦Ï€ interactions between CH3CN/CH3NC and H2O, NH3 or C2H2: A B3LYP and MP2 theoretical study. Computational and Theoretical Chemistry, 2008, 849, 76-83.	1.5	15
60	Can BB double bond be as potential proton acceptor: A UB3LYP and UMP2 theoretical study on unusual intermolecular T-shaped XHâ€¦Ï€ interactions between the triplet state HBBH and HF, HCl, HCN or H2C2. Computational and Theoretical Chemistry, 2008, 870, 43-48.	1.5	16