

Fu-de Ren

List of Publications by Year in descending order

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papers

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#	ARTICLE	IF	CITATIONS
1	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). <i>Computational Materials Science</i> , 2015, 107, 33-41.	1.4	46
2	Theoretical insight into the binding energy and detonation performance of $\hat{\mu}$ -, $\hat{\nu}$ -, $\hat{\omega}$ -CL-20 cocrystals with $\hat{\nu}$ -HMX, FOX-7, and DMF in different molar ratios, as well as electrostatic potential. <i>Journal of Molecular Modeling</i> , 2016, 22, 123.	0.8	35
3	A theoretical prediction of the possible trigger linkage of CH ₃ NO ₂ and NH ₂ NO ₂ in an external electric field. <i>Journal of Molecular Modeling</i> , 2015, 21, 145.	0.8	29
4	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. <i>Journal of Molecular Modeling</i> , 2015, 21, 245.	0.8	27
5	Theoretical Insight into the Influences of Molecular Ratios on Stabilities and Mechanical Properties, Solvent Effect of HMX/FOX-7 Cocrystal Explosive. <i>Journal of Energetic Materials</i> , 2016, 34, 426-439.	1.0	25
6	Growth morphology of CL-20/HMX cocrystal explosive: insights from solvent behavior under different temperatures. <i>Journal of Molecular Modeling</i> , 2017, 23, 360.	0.8	25
7	A dynamic prediction of stability for nitromethane in external electric field. <i>RSC Advances</i> , 2017, 7, 47063-47072.	1.7	22
8	Molecular dynamics simulation and density functional theory insight into the cocrystal explosive of hexaazaisowurtzitane/nitroguanidine. <i>International Journal of Quantum Chemistry</i> , 2016, 116, 88-96.	1.0	21
9	Can BB triple bond be as potential proton acceptor: An ab initio study on unusual intermolecular T-shaped X $\hat{\nu}$ -H $\hat{\nu}$ - $\hat{\nu}$ interactions between OCBBCO and HF, HCl, HCN or H ₂ C ₂ . <i>Chemical Physics Letters</i> , 2008, 455, 32-37.	1.2	19
10	A dynamics prediction of nitromethane $\hat{\nu}$ methyl nitrite isomerization in external electric field. <i>Journal of Molecular Modeling</i> , 2016, 22, 96.	0.8	19
11	A theoretical study on unusual intermolecular T-shaped X $\hat{\nu}$ -H... $\hat{\nu}$ interactions between the singlet state HB=BH and HF, HCl, HCN or H ₂ C ₂ . <i>Journal of Molecular Modeling</i> , 2009, 15, 515-523.	0.8	17
12	Can BB double bond be as potential proton acceptor: A UB3LYP and UMP2 theoretical study on unusual intermolecular T-shaped XH $\hat{\nu}$ - $\hat{\nu}$ interactions between the triplet state HBBH and HF, HCl, HCN or H ₂ C ₂ . <i>Computational and Theoretical Chemistry</i> , 2008, 870, 43-48.	1.5	16
13	Unusual intermolecular T-shaped X $\hat{\nu}$ -H $\hat{\nu}$ - $\hat{\nu}$ interactions between CH ₃ CN/CH ₃ NC and H ₂ O, NH ₃ or C ₂ H ₂ : A B3LYP and MP2 theoretical study. <i>Computational and Theoretical Chemistry</i> , 2008, 849, 76-83.	1.5	15
14	A MP2(full) and CCSD(T) theoretical investigation on unusual cation $\hat{\nu}$ - $\hat{\nu}$ interaction between OCBBCO and H ⁺ , Li ⁺ , Na ⁺ , Be ²⁺ or Mg ²⁺ . <i>Computational and Theoretical Chemistry</i> , 2009, 913, 221-227.	1.5	14
15	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 ⁺ , Be ²⁺ or Mg ²⁺ . <i>Journal of Molecular Modeling</i> , 2012, 18, 2105-2115.	0.8	13
16	Theoretical investigation of the effects of the molar ratio and solvent on the formation of the pyrazole $\hat{\nu}$ -nitroamine cocrystal explosive 3,4-dinitropyrazole (DNP)/2,4,6,8,10,12-hexanitrohexaazaisowurtzitane (CL-20). <i>Journal of Molecular Modeling</i> , 2017, 23, 353.	0.8	13
17	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 XH $\hat{\nu}$ - $\hat{\nu}$ interaction between HF and HBBH ($\hat{\nu}$), HBBH (1 $\hat{\nu}$ g), OCBBCO, H ₂ CCH ₂ or HCCH. <i>Computational and Theoretical Chemistry</i> , 2009, 896, 38-43.	1.5	12
18	Theoretical investigation on geometries and aromaticity of mixed boron-, nitrogen- and furanoxo-containing five-membered rings B ₂ N ₂ OHp (p=0 $\hat{\nu}$ 2). <i>Computational and Theoretical Chemistry</i> , 2009, 909, 13-18.	1.5	12

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19	A UB3LYP and UMP2 theoretical investigation on unusual cation-π interaction between the triplet state HB=BH (σ_g^3) and H+, Li+, Na+, Be2+ or Mg2+. Journal of Molecular Modeling, 2010, 16, 615-627.	0.8	12
20	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
21	A B3LYP and MP2 theoretical investigation on unusual cation-π interaction between the singlet state HBBH (1 ^g) and H+, Li+, Na+, Be2+ or Mg2+. Computational and Theoretical Chemistry, 2009, 909, 79-85.	1.5	11
22	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
23	A B3LYP and MP2(full) theoretical investigation into explosive sensitivity upon the formation of the intermolecular hydrogen-bonding interaction between the nitro group of RNO ₂ (R=CH ₃ , NH ₂), Tj ETQq1 1 0.784314 rBT / Overlock 10 Tf		
24	A B3LYP and MP2(full) theoretical investigation on the cooperativity effect between cation-π molecule and hydrogen-bonding interactions in the O-cresol complex with Na+. Computational and Theoretical Chemistry, 2012, 996, 91-102.	1.1	11
25	A B3LYP and MP2(full) theoretical investigation into the strength of the C-NO ₂ 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
26	Theoretical insights into the stabilities, detonation performance, and electrostatic potentials of cocrystals containing 1 [±] - or 1 ² -HMX and TATB, FOX-7, NTO, or DMF in various molar ratios. Journal of Molecular Modeling, 2016, 22, 249.	0.8	10
27	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
28	Theoretical insight into the BH ₃ -HCN adsorption on the Co(100) and Co(110) surfaces as hydrogen storage. Journal of Molecular Modeling, 2017, 23, 126.	0.8	10
29	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
30	A (U)MP2(full) and (U)CCSD(T) theoretical investigation on the substituent effect on the cation-π interactions between Na+ and LCCL (L=H, CH ₃ , OH, F, Cl, CO, NN, CN ⁺ , NC ⁺ and OH ⁺). Computational and Theoretical Chemistry, 2010, 956, 1-9.	1.5	8
31	A theoretical study on the strength of the C-NO ₂ 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
32	A MP2(full) theoretical investigation on the π-halogen interaction between OCBBCO and X1X2 (X1, X2) Tj ETQq0 0 0 rBT / Overlock 10 Tf		
33	A MP2 and CCSD(T) theoretical investigation on the weak dihydrogen-bonded interactions between HBBH (1 ^g) and HM (M=Li, Na, K, BeH, MgH or CaH). Computational and Theoretical Chemistry, 2011, 963, 463-469.	1.1	7
34	External electric field reduces the explosive sensitivity: a theoretical investigation into the hydrogen transference kinetics of the NH ₂ NO ₂ -H ₂ O complex. Journal of Molecular Modeling, 2020, 26, 351.	0.8	7
35	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
36	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

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37	Can the positive aromatic ring be as π -electron donor in π -halogen bond? A MP2 theoretical investigation on the unusual π -halogen bond interaction between three-membered ring C_2H_2 , C_2H_4 or C_6H_6 . <i>Journal of Molecular Modeling</i> , 2013, 19, 929-937.	0.8	6
38	A dynamic and electrostatic potential prediction of the prototropic tautomerism between imidazole 3-oxide and 1-hydroxyimidazole in external electric field. <i>Journal of Molecular Modeling</i> , 2019, 25, 330.	0.8	6
39	A B3LYP and MP2(full) theoretical investigation into the strength of the C-NO ₂ bond upon the formation of the molecule-cation interaction between Na ⁺ and the nitro group of nitrotriazole or its methyl derivatives. <i>Journal of Molecular Modeling</i> , 2013, 19, 453-463.	0.8	5
40	A B3LYP and MP2(full) theoretical investigation into the cooperativity effect between dihydrogen-bonding and H π - π interactions among HF, MH with the π -electron donor C_2H_2 , C_2H_4 or C_6H_6 . <i>Journal of Molecular Modeling</i> , 2013, 19, 3153-3163.	0.8	4
41	A theoretical investigation into the strength of N π -NO ₂ bonds, ring strain and electrostatic potential upon formation of intermolecular H-bonds between HF and the nitro group in nitrogen heterocyclic rings $\text{C}_n\text{H}_{2n}\text{N}\pi\text{-NO}_2$ ($n=2-5$), RDX and HMX. <i>Journal of Molecular Modeling</i> , 2015, 21, 302.	0.8	4
42	Theoretical prediction of the impact sensitivities of energetic C-nitro compounds. <i>Journal of Molecular Modeling</i> , 2020, 26, 219.	0.8	4
43	A theoretical investigation into the cooperativity effect on the TNT melting point under external electric field. <i>Journal of Molecular Modeling</i> , 2021, 27, 4.	0.8	4
44	A B3LYP and MP2(full) theoretical investigation into explosive sensitivity upon the formation of the molecule-cation interaction between the nitro group of RNO ₂ (R= π -CH ₃ , π -NH ₂ , π -OCH ₃) and Na ⁺ , Mg ²⁺ or Al ³⁺ . <i>Computational and Theoretical Chemistry</i> , 2012, 991, 107-115.	1.1	3
45	Theoretical investigation of the safety of nitroguanidine-based PBXs containing the nonpolar desensitizing agent polytetrafluoroethylene. <i>Journal of Molecular Modeling</i> , 2017, 23, 346.	0.8	3
46	Theoretical investigation into the cooperativity effect between the intermolecular π - π and H-bonding interactions in the curcumin π -cytosine π -H ₂ O system. <i>Journal of Molecular Modeling</i> , 2018, 24, 298.	0.8	3
47	Cooperativity effect of the π - π interaction between drug and DNA on intercalative binding induced by H-bonds: a QM/QTAIM investigation of the curcumin π -adenine π -H ₂ O model system. <i>Physical Chemistry Chemical Physics</i> , 2019, 21, 11871-11882.	1.3	3
48	Theoretical evaluation to improve the performance of composite wax powder: cooperativity effects involving the strong Na ⁺ - π and weak hydrogen-bonding interactions in the complex of graphene oxide with Na ⁺ and CH ₄ . <i>Molecular Physics</i> , 2020, 118, e1612106.	0.8	3
49	A comparative theoretical investigation into the strength of the trigger-bond in the Na ⁺ , Mg ²⁺ and HF complexes involving the nitro group of R π -NO ₂ (R= π -CH ₃ , π -NH ₂ and π -OCH ₃) or the C π -O bond of (E)-O ₂ N π -CH π -NO ₂ . <i>Journal of Molecular Modeling</i> , 2013, 19, 2499-2507.	0.8	3
50	Theoretical insight into the sensitive mechanism of multilayer-shaped cocrystal explosives: compression and slide. <i>Journal of Molecular Modeling</i> , 2016, 22, 108.	0.8	2
51	Theoretical explanation for the DNA cleavage by GO with cation: anti-cooperativity effect among the π - π , cation π and H-bonding interactions in cytosine π -GO π -M ⁿ⁺ (M ⁿ⁺ =Na ⁺ , Mg ²⁺ , Al ³⁺). <i>Molecular Physics</i> , 2020, 118, e1692149.	0.8	2
52	Hydration and swelling: a theoretical investigation on the cooperativity effect of H-bonding interactions between p-hydroxy hydroxymethyl calix[4]/[5]arene and H ₂ O by many-body interaction and density functional reactivity theory. <i>Journal of Molecular Modeling</i> , 2020, 26, 190.	0.8	2
53	Theoretical investigation on the structures and thermodynamic properties of mixed boron-, nitrogen- and oxygen-containing three- and four-membered rings B _n N _m O _p (n=0-3, m=0-3, p=0-3). <i>Computational and Theoretical Chemistry</i> , 2010, 942, 121-130.	1.5	1
54	A (U)MP2(full) and (U)CCSD(T) theoretical investigation into the substituent effects on the cation π interactions between M ⁺ (M=Li or Na) and LBBL (L=H, CH ₃ , OH, CN, NC, F, :CO, :NN, :BH, :CN π , :NC π) <i>Journal of Molecular Modeling</i> , 2010, 16, 100-108.	0.8	1

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55	A (U)MP2(full) and (U)CCSD(T) theoretical investigation into the substituent effects on the intermolecular T-shaped F-H...I interactions between HF and LBBL (L = H, CO, :NN, Cl, CN and NO). Journal of Molecular Modeling, 2012, 18, 2959-2969.		1
56	A B3LYP AND MP2(FULL) THEORETICAL INVESTIGATION INTO THE NO ₂ 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
57	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
58	Theoretical investigation into the cooperativity effect of 1,4-dimethoxy-d-glucosamine complex with Na ⁺ and H ₂ O. Journal of Molecular Modeling, 2020, 26, 203.	0.8	1
59	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
60	A correction into 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, 352.	0.8	0