

# Computer simulation for prediction of performance and high energy materials

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Citation Report

#	ARTICLE	IF	CITATIONS
2	Prediction of heat of formation and related parameters of high energy materials. Journal of Hazardous Materials, 2006, 133, 30-45.	6.5	67
3	Computer code for the optimization of performance parameters of mixed explosive formulations. Journal of Hazardous Materials, 2006, 136, 475-481.	6.5	20
4	Synthesis, characterization and thermolysis studies on new derivatives of 2,4,5-trinitroimidazoles: Potential insensitive high energy materials. Journal of Hazardous Materials, 2007, 143, 192-197.	6.5	75
5	Globally convergent computation of chemical equilibrium composition. Journal of Computational Chemistry, 2008, 29, 1032-1036.	1.5	0
6	Synthesis, characterization and thermolysis studies on 3,7-dinitro-1,3,5,7-tetraazabicyclo[3,3,1]nonane (DPT): A key precursor in the synthesis of most powerful benchmark energetic materials (RDX/HMX) of today. Journal of Hazardous Materials, 2008, 152, 1317-1324.	6.5	23
7	New Atom/Group Volume Additivity Method to Compensate for the Impact of Strong Hydrogen Bonding on Densities of Energetic Materials. Journal of Chemical & Engineering Data, 2008, 53, 520-524.	1.0	57
8	Modeling Growth, Surface Kinetics, and Morphology Evolution in PETN. Propellants, Explosives, Pyrotechnics, 2009, 34, 489-497.	1.0	22
9	Computer code to predict the heat of explosion of high energy materials. Journal of Hazardous Materials, 2009, 161, 714-717.	6.5	11
10	Synthesis and characterization of 3,6-bis(1H-1,2,3,4-tetrazol-5-ylamino)-1,2,4,5-tetrazine (BTATz): Novel high-nitrogen content insensitive high energy material. Journal of Hazardous Materials, 2009, 170, 306-313.	6.5	53
11	Synthesis, characterization and evaluation of 1,2-bis(2,4,6-trinitrophenyl) hydrazine: A key precursor for the synthesis of high performance energetic materials. Journal of Hazardous Materials, 2009, 172, 276-279.	6.5	17
12	A new computer code to evaluate detonation performance of high explosives and their thermochemical properties, part I. Journal of Hazardous Materials, 2009, 172, 1218-1228.	6.5	64
13	MATEO: A software package for the molecular design of energetic materials. Journal of Hazardous Materials, 2010, 176, 313-322.	6.5	15
14	Simple Pathway to Predict the Power of High Energy Materials. Propellants, Explosives, Pyrotechnics, 2011, 36, 424-429.	1.0	12
15	A transportable fast neutron and dual gamma-ray system for the detection of illicit materials. Nuclear Instruments and Methods in Physics Research, Section A: Accelerators, Spectrometers, Detectors and Associated Equipment, 2011, 648, 275-284.	0.7	9
16	A new approach to predict the strength of high energy materials. Journal of Hazardous Materials, 2011, 186, 175-181.	6.5	9
17	Characterization and Properties of a Novel Energetic "Energetic Cocrystal Explosive Composed of HNIW and BTF. Crystal Growth and Design, 2012, 12, 5155-5158.	1.4	226
18	A Simple Way to Predict Heats of Detonation of Energetic Compounds only from Their Molecular Structures. Propellants, Explosives, Pyrotechnics, 2012, 37, 93-99.	1.0	14
19	Predicting Maximum Attainable Detonation Velocity of CHNOF and Aluminized Explosives. Propellants, Explosives, Pyrotechnics, 2012, 37, 489-497.	1.0	15

#	ARTICLE	IF	CITATIONS
20	PtII6 nanoscopic cages with an organometallic backbone as sensors for picric acid. Dalton Transactions, 2013, 42, 16784.	1.6	62
21	Preparation and Performance of a HNIW/TNT Cocrystal Explosive. Propellants, Explosives, Pyrotechnics, 2013, 38, 495-501.	1.0	90
22	Multiple fast neutron and gamma-ray beam systems for the detection of illicit materials. Journal of Radioanalytical and Nuclear Chemistry, 2013, 295, 973-977.	0.7	2
23	A New Computer Code for Assessment of Energetic Materials with Crystal density, Condensed Phase Enthalpy of Formation, and Activation Energy of Thermolysis. Propellants, Explosives, Pyrotechnics, 2013, 38, 95-102.	1.0	33
24	Fluorescent Tris-Imidazolium Sensors for Picric Acid Explosive. Journal of Organic Chemistry, 2013, 78, 1306-1310.	1.7	240
25	ICT-not-quenching near infrared ratiometric fluorescent detection of picric acid in aqueous media. Chemical Communications, 2013, 49, 4764.	2.2	178
26	The Pyreno-Triazinyl Radical Magnetic and Sensor Properties. Israel Journal of Chemistry, 2014, 54, 774-778.	1.0	50
27	Cocrystal explosive hydrate of a powerful explosive, HNIW, with enhanced safety. RSC Advances, 2014, 4, 65121-65126.	1.7	40
28	Preparation and Performance of a BTF/DNB Cocrystal Explosive. Propellants, Explosives, Pyrotechnics, 2014, 39, 9-13.	1.0	49
29	A Novel Cocrystal Explosive of HNIW with Good Comprehensive Properties. Propellants, Explosives, Pyrotechnics, 2014, 39, 590-596.	1.0	120
30	Crystal Packing of Low-Sensitivity and High-Energy Explosives. Crystal Growth and Design, 2014, 14, 4703-4713.	1.4	276
31	Evident Hydrogen Bonded Chains Building CL-20-Based Cocrystals. Crystal Growth and Design, 2014, 14, 3923-3928.	1.4	54
32	Complex Formation-Enhanced Fluorescence Quenching Effect for Efficient Detection of Picric Acid. Chemistry - A European Journal, 2014, 20, 12215-12222.	1.7	78
33	Rhodamine based selective turn-on sensing of picric acid. RSC Advances, 2014, 4, 30828-30831.	1.7	150
34	Prediction of Sensitivity of Energetic Compounds with a New Computer Code. Propellants, Explosives, Pyrotechnics, 2014, 39, 95-101.	1.0	22
35	A Fluorescent 1,3-Diaminonaphthalimide Conjugate of Calix[4]arene for Sensitive and Selective Detection of Trinitrophenol: Spectroscopy, Microscopy, and Computational Studies, and Its Applicability using Cellulose Strips. Chemistry - A European Journal, 2015, 21, 13364-13374.	1.7	44
36	Study on the Azido-Tetrazolo Tautomerizations of 3,6-Bis(azido)-1,2,4,5-tetrazine. Propellants, Explosives, Pyrotechnics, 2015, 40, 627-631.	1.0	8
37	Assessment of the Strength of Energetic Compounds Through the Trauzl Lead Block Expansions Using Their Molecular Structures. Zeitschrift Fur Anorganische Und Allgemeine Chemie, 2015, 641, 2446-2451.	0.6	7

#	ARTICLE	IF	CITATIONS
38	Identifying high energy molecules and predicting their detonation potency using chemometric modelling approaches. <i>Combustion Theory and Modelling</i> , 2015, 19, 451-464.	1.0	4
39	Cubane: 50 Years Later. <i>Chemical Reviews</i> , 2015, 115, 6719-6745.	23.0	145
40	A suitable computer code for prediction of sublimation energy and deflagration temperature of energetic materials. <i>Journal of Thermal Analysis and Calorimetry</i> , 2015, 121, 675-681.	2.0	13
41	Prediction of heats of sublimation of energetic compounds using their molecular structures. <i>Journal of Thermal Analysis and Calorimetry</i> , 2015, 120, 1941-1951.	2.0	37
42	Electron-Rich Triphenylamine-Based Sensors for Picric Acid Detection. <i>Journal of Organic Chemistry</i> , 2015, 80, 4064-4075.	1.7	145
43	1,8-Naphthyridine-based fluorescent receptors for picric acid detection in aqueous media. <i>Analytical Methods</i> , 2015, 7, 10272-10279.	1.3	31
44	Aggregates of a hydrazone-sulfonamide adduct as picric acid sensors. <i>RSC Advances</i> , 2015, 5, 92473-92479.	1.7	20
45	Electron-rich $\pi$ -extended phthalocyanine- $\pi$ -thiophene- $\pi$ -phthalocyanine triad for the sensitive and selective detection of picric acid. <i>RSC Advances</i> , 2015, 5, 73989-73992.	1.7	11
46	A novel high-energetic and good-sensitive cocrystal composed of CL-20 and TATB by a rapid solvent/non-solvent method. <i>RSC Advances</i> , 2015, 5, 95764-95770.	1.7	72
47	Concentration dependent ratiometric turn-on selective fluorescence detection of picric acid in aqueous and non-aqueous media. <i>RSC Advances</i> , 2015, 5, 3903-3907.	1.7	10
48	A New Computer Code for Prediction of Enthalpy of Fusion and Melting Point of Energetic Materials. <i>Propellants, Explosives, Pyrotechnics</i> , 2015, 40, 150-155.	1.0	18
49	A novel heteroacene 2-(perfluorophenyl)-1H-imidazo[4,5-b]phenazine for selective sensing of picric acid. <i>RSC Advances</i> , 2016, 6, 37929-37932.	1.7	17
50	Recent Developments for Prediction of Power of Aromatic and Non-Aromatic Energetic Materials along with a Novel Computer Code for Prediction of Their Power. <i>Propellants, Explosives, Pyrotechnics</i> , 2016, 41, 942-948.	1.0	3
51	Fluorescence tuning of Zn(II)-based metallo-supramolecular coordination polymers and their application for picric acid detection. <i>Inorganic Chemistry Frontiers</i> , 2016, 3, 1363-1375.	3.0	25
52	Comparative study of melting points of 3,4-bis(3-nitrofurazan-4-yl)furoxan (DNTF)/1,3,3-trinitroazetidine (TNAZ) eutectic compositions using molecular dynamic simulations. <i>RSC Advances</i> , 2016, 6, 59141-59149.	1.7	23
53	Charge-Transfer-Induced Fluorescence Quenching of Anthracene Derivatives and Selective Detection of Picric Acid. <i>Chemistry - A European Journal</i> , 2016, 22, 2012-2019.	1.7	106
54	Highly sensitive fluorescent imidazolium-based sensors for nanomolar detection of explosive picric acid in aqueous medium. <i>Sensors and Actuators B: Chemical</i> , 2016, 229, 599-608.	4.0	70
55	Perylene Diimide Based Fluorescent Dyes for Selective Sensing of Nitroaromatic Compounds: Selective Sensing in Aqueous Medium Across Wide pH Range. <i>Journal of Fluorescence</i> , 2016, 26, 395-401.	1.3	25

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56	Theoretical insights into the effects of molar ratios on stabilities, mechanical properties, and detonation performance of CL-20/HMX cocrystal explosives by molecular dynamics simulation. <i>Journal of Molecular Modeling</i> , 2017, 23, 30.	0.8	16
57	Structurally modified RDX - A DFT study. <i>Defence Technology</i> , 2017, 13, 385-391.	2.1	12
58	A Highly Selective Fluorescent Chemosensor for the Detection of Picrate Anion Based on 1,8-Naphthalimide Derivatives. <i>Journal of Applied Spectroscopy</i> , 2017, 84, 25-30.	0.3	16
59	Theoretical insights into effects of molar ratios on stabilities, mechanical properties and detonation performance of CL-20/RDX cocrystal explosives by molecular dynamics simulation. <i>Journal of Molecular Structure</i> , 2017, 1141, 577-583.	1.8	29
60	A nonconjugated macromolecular luminogen for speedy, selective and sensitive detection of picric acid in water. <i>Polymer Chemistry</i> , 2017, 8, 7180-7187.	1.9	58
61	Ultrasensitive detection of explosives via hydrophobic condensation effect on biomimetic SERS platforms. <i>Journal of Materials Chemistry C</i> , 2017, 5, 12384-12392.	2.7	41
62	Molecular dynamics calculation on structures, stabilities, mechanical properties, and energy density of CL-20/FOX-7 cocrystal explosives. <i>Journal of Molecular Modeling</i> , 2017, 23, 362.	0.8	8
63	Metal-free Unsaturated Ketothiolester: Solvatochromism, AIEE and Detection of Picric Acid. <i>ChemistrySelect</i> , 2018, 3, 4075-4081.	0.7	8
64	Synthesis, Crystal Structure, and Thermal Behavior of a Novel Insensitive Energetic Cocrystal Composed of 3,3'-Bis(1,2,4-oxadiazole)-5,5'-dione and 4-Amino-1,2,4-triazole. <i>Zeitschrift Fur Anorganische Und Allgemeine Chemie</i> , 2018, 644, 466-471.		8
65	5-Nitro-2,4-Dihydro-3H-1,2,4-Triazole-3-One (NTO). , 2018, , 163-211.		3
66	Novel 2-Arylbenzothiazoles: Selective Chromogenic and Fluorescent Probes for the Detection of Picric Acid. <i>ChemistrySelect</i> , 2018, 3, 4598-4608.	0.7	15
67	Investigation on sensing mechanism of a fluorescent probe for TNP detection in aqueous solution. <i>Tetrahedron</i> , 2018, 74, 2684-2691.	1.0	21
68	Fluorescent nanoaggregates of quinoxaline derivatives for highly efficient and selective sensing of trace picric acid. <i>Dyes and Pigments</i> , 2018, 155, 107-113.	2.0	41
76	Assessment of density prediction methods based on molecular surface electrostatic potential. <i>Journal of Molecular Modeling</i> , 2018, 24, 166.	0.8	10
77	Theoretical investigations on stabilities, sensitivity, energetic performance and mechanical properties of CL-20/NTO cocrystal explosives by molecular dynamics simulation. <i>Theoretical Chemistry Accounts</i> , 2018, 137, 1.	0.5	17
78	Shock response of condensed-phase RDX: molecular dynamics simulations in conjunction with the MSST method. <i>RSC Advances</i> , 2018, 8, 17312-17320.	1.7	12
79	Synthesis, spectral, and computational studies of some energetic picrates. <i>Journal of Molecular Structure</i> , 2019, 1195, 378-386.	1.8	3
80	Syntheses, Crystal Structures, and Properties of Two Novel CL-20-based Cocrystals. <i>Zeitschrift Fur Anorganische Und Allgemeine Chemie</i> , 2019, 645, 656-662.	0.6	13

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81	Effect of external growth environment on cocrystal habits of HNIW/DNB: a molecular dynamics simulation. <i>Canadian Journal of Chemistry</i> , 2020, 98, 746-754.	0.6	0
82	Intermolecular interactions, vibrational spectra, and detonation performance of CL-20/TNT cocrystal. <i>Journal of the Chinese Chemical Society</i> , 2020, 67, 1742-1752.	0.8	9
83	Machine-Learning Assisted Screening of Energetic Materials. <i>Journal of Physical Chemistry A</i> , 2020, 124, 5341-5351.	1.1	37
84	Design of new energetic materials based on derivatives of 1,3,5-trinitrobenzenes: A theoretical and computational prediction of detonation properties, blast impulse and combustion parameters. <i>Heliyon</i> , 2020, 6, e03163.	1.4	7
85	High-efficiency fluorescent probe constructed by triazine polycarboxylic acid for detecting nitro compounds. <i>Inorganica Chimica Acta</i> , 2020, 507, 119591.	1.2	12
86	Different Stoichiometric Ratios Realized in Energetic Energetic Cocrystals Based on CL-20 and 4,5-MDNI: A Smart Strategy to Tune Performance. <i>Crystal Growth and Design</i> , 2020, 20, 3826-3833.	1.4	28
87	Density Prediction Models for Energetic Compounds Merely Using Molecular Topology. <i>Journal of Chemical Information and Modeling</i> , 2021, 61, 2582-2593.	2.5	25
88	Magic of Numbers: A Guide for Preliminary Estimation of the Detonation Performance of Explosives Based on Empirical Formulas. <i>Industrial &amp; Engineering Chemistry Research</i> , 2021, 60, 1952-1961.	1.8	13
89	ON THE EXPLICIT DETERMINATION OF THE CHAPMAN-JOUQUET PARAMETERS FOR AN EXPLOSIVE COMPOUND. <i>International Journal of Energetic Materials and Chemical Propulsion</i> , 2015, 14, 125-145.	0.2	1
90	Efficient detection of Picric acid by pyranone based Schiff base as a chemosensor. <i>Journal of Molecular Structure</i> , 2022, 1249, 131619.	1.8	19
91	Multi-Level Structural Design Strategy toward Low-Sensitivity Energetic Materials: From Planar Molecule to Layered Packing Crystal. <i>Crystal Growth and Design</i> , 2022, 22, 1882-1891.	1.4	4
92	Simple Model for Predicting the Detonation Velocity of Organic, Inorganic, and Mixed Explosives. <i>Combustion, Explosion and Shock Waves</i> , 2021, 57, 726-735.	0.3	1
93	Silver(I)-Carbene Bond-Directed Rigidification-Induced Emissive Metallacage for Picric Acid Detection. <i>Inorganic Chemistry</i> , 2022, 61, 713-722.	1.9	26
94	Theoretical Calculation of Cocrystal Components for Explosives: A Similarity Function of Energetic Supramolecules. <i>Crystal Growth and Design</i> , 2022, 22, 293-303.	1.4	2
95	Solubility Determination, Computational Methodologies, and Preferential Solvation of 3-Nitro-1,2,4-triazol-5-one in Several Solvent Blends. <i>Journal of Chemical &amp; Engineering Data</i> , 0, , .	1.0	1
96	Computational Evaluation of Polycyclic Bis-Oxadiazolo-Pyrazine Backbone in Designing Potential Energetic Materials. <i>Polycyclic Aromatic Compounds</i> , 2023, 43, 6717-6729.	1.4	0
97	The Effects of BTTN, TMETN and DEGDN Molecules on the Explosion Properties of PETN Molecule. <i>Journal of Natural and Applied Sciences</i> , 2022, 26, 366-371.	0.1	0
98	Triazole-based pyrene-sugar analogues for selective detection of picric acid in water medium and paper strips. <i>Journal of Photochemistry and Photobiology A: Chemistry</i> , 2023, 440, 114647.	2.0	6

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99	Methods for Detecting Picric Acid—A Review of Recent Progress. Applied Sciences (Switzerland), 2023, 13, 3991.	1.3	6