Maija M Kuklja

List of Publications by Year
in descending order

76	2,626	117625	189892
papers	citations	34 h-index	50 g-index

76	76	76	1713
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	An excitonic mechanism of detonation initiation in explosives. Journal of Chemical Physics, 2000, 112, 3417-3423.	3.0	162
2	Role of electronic excitations in explosive decomposition of solids. Journal of Applied Physics, 2001, 89, 4156-4166.	2.5	120
3	Formation and migration of oxygen vacancies in La_{1â^'x}Sr_xCo_{1â^'y}Fe_yO_{3â^'Î´}perovskites: insight from ab initio calculations and comparison with Ba_{1â^'x}Sr_xCo_{1â^'y}Fe_yO_{3â^'Î´}. Physical Chemistry Chemical Physics, 2013, 15, 911-918.	2.8	111
4	Shear-strain-induced chemical reactivity of layered molecular crystals. Applied Physics Letters, 2007, 90, 151913.	3.3	97
5	Laser Initiation of Energetic Materials: Selective Photoinitiation Regime in Pentaerythritol Tetranitrate. Journal of Physical Chemistry C, 2011, 115, 6893-6901.	3.1	90
6	First Principles Calculations of Oxygen Vacancy Formation and Migration in Ba_{1â^'x}Sr_xCo_{1â^'y}Fe_yO_{3â^'Î´}Perovskites. Journal of the Electrochemical Society, 2011, 159, B219-B226.	2.9	84
7	First-principles modelling of complex perovskite (Ba1-xSrx)(Co1-yFey)O3-Î´ for solid oxide fuel cell and gas separation membrane applications. Energy and Environmental Science, 2010, 3, 1544.	30.8	75
8	Ab initio simulation of defects in energetic materials: Hydrostatic compression of cyclotrimethylene trinitramine. Journal of Applied Physics, 1999, 86, 4428-4434.	2.5	73
9	Modeling Thermal Decomposition Mechanisms in Gaseous and Crystalline Molecular Materials: Application to Î²-HMX. Journal of Physical Chemistry B, 2011, 115, 12677-12686.	2.6	66
10	Adsorption of Dimethyl Methylphosphonate on MoO₃: The Role of Oxygen Vacancies. Journal of Physical Chemistry C, 2016, 120, 29077-29088.	3.1	66
11	Rapid Materials Degradation Induced by Surfaces and Voids: Ab Initio Modeling of Î²-Octatetramethylene Tetranitramine. Journal of the American Chemical Society, 2012, 134, 11815-11820.	13.7	65
12	Searching for Low-Sensitivity Cast-Melt High-Energy-Density Materials: Synthesis, Characterization, and Decomposition Kinetics of 3,4-Bis(4-nitro-1,2,5-oxadiazol-3-yl)-1,2,5-oxadiazole-2-oxide. Journal of Physical Chemistry C, 2015, 119, 3509-3521.	3.1	64
13	Molecular Theory of Detonation Initiation: Insight from First Principles Modeling of the Decomposition Mechanisms of Organic Nitro Energetic Materials. Molecules, 2016, 21, 236.	3.8	61
14	Electronic structure of molecular crystals containing edge dislocations. Journal of Applied Physics, 2001, 89, 4962-4970.	2.5	58
15	Compression-induced effect on the electronic structure of cyclotrimethylene trinitramine containing an edge dislocation. Journal of Applied Physics, 2000, 87, 2215-2218.	2.5	57
16	Shear-strain-induced structural and electronic modifications of the molecular crystal 1,1-diamino-2,2-dinitroethylene: Slip-plane flow and band gap relaxation. Physical Review B, 2007, 75, .	3.2	56
17	The Intrinsic Defects, Disordering, and Structural Stability of Ba_xSr_{1â€“x}Co_yFe_{1â€“y}O_{3â^'Î´} Perovskite Solid Solutions. Journal of Physical Chemistry C, 2012, 116, 18605-18611.	3.3	56
18	Adsorption and Destruction of the G-Series Nerve Agent Simulant Dimethyl Methylphosphonate on Zinc Oxide. ACS Catalysis, 2019, 9, 902-911.	11.2	54

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19	Effect of Molecular and Lattice Structure on Hydrogen Transfer in Molecular Crystals of Diamino-dinitroethylene and Triamino-trinitrobenzene. Journal of Physical Chemistry A, 2008, 112, 4496-4500.	2.5	53
20	Surface-Enhanced Decomposition Kinetics of Molecular Materials Illustrated with Cyclotetramethylene-tetranitramine. Journal of Physical Chemistry C, 2012, 116, 11077-11081.	3.1	52
21	Effect of charged and excited states on the decomposition of 1,1-diamino-2,2-dinitroethylene molecules. Journal of Chemical Physics, 2007, 126, 234711.	3.0	50
22	Interplay of Decomposition Mechanisms at Shear-Strain Interface. Journal of Physical Chemistry C, 2009, 113, 17-20.	3.1	49
23	Understanding Limits of the Thermal Mechanism of Laser Initiation of Energetic Materials. Journal of Physical Chemistry C, 2012, 116, 24482-24486.	3.1	49
24	Surface-Accelerated Decomposition of Î´-HMX. Journal of Physical Chemistry Letters, 2013, 4, 730-734.	4.6	49
25	Spectroscopic and Computational Investigation of Room-Temperature Decomposition of a Chemical Warfare Agent Simulant on Polycrystalline Cupric Oxide. Chemistry of Materials, 2017, 29, 7483-7496.	6.7	48
26	Simulation of Defects in Energetic Materials. 3. The Structure and Properties of RDX Crystals with Vacancy Complexes. Journal of Physical Chemistry B, 1999, 103, 8427-8431.	2.6	47
27	Atomistic Modeling of Native Point Defects in Yttrium Aluminum Garnet Crystals. Journal of the American Ceramic Society, 1999, 82, 2881-2886.	3.8	47
28	Effect of Polar Surfaces on Decomposition of Molecular Materials. Journal of the American Chemical Society, 2014, 136, 13289-13302.	13.7	44
29	Comprehensive End-to-End Design of Novel High Energy Density Materials: I. Synthesis and Characterization of Oxadiazole Based Heterocycles. Journal of Physical Chemistry C, 2017, 121, 23853-23864.	3.1	42
30	Thermal Decomposition Mechanisms of Nitroesters: Ab Initio Modeling of Pentaerythritol Tetranitrate. Journal of Physical Chemistry C, 2013, 117, 18144-18153.	3.1	41
31	Ab Initio Kinetics of Gas Phase Decomposition Reactions. Journal of Physical Chemistry A, 2010, 114, 12656-12661.	2.5	40
32	Initiation of chemistry in molecular solids by processes involving electronic excited states. Thermochimica Acta, 2002, 384, 279-284.	2.7	38
33	Surface termination effects on the oxygen reduction reaction rate at fuel cell cathodes. Journal of Materials Chemistry A, 2018, 6, 11929-11940.	10.3	38
34	Self-Accelerated Mechanochemistry in Nitroarenes. Journal of Physical Chemistry Letters, 2010, 1, 363-367.	4.6	35
35	Decomposition Mechanisms and Kinetics of Novel Energetic Molecules BNFF-1 and ANFF-1: Quantum-Chemical Modeling. Molecules, 2013, 18, 8500-8517.	3.8	34
36	Comprehensive End-To-End Design of Novel High Energy Density Materials: III. Fused Heterocyclic Energetic Compounds. Journal of Physical Chemistry C, 2019, 123, 8688-8698.	3.1	29

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37	Synthetic Crystals of Silver with Carbon: 3D Epitaxy of Carbon Nanostructures in the Silver Lattice. Advanced Functional Materials, 2015, 25, 4768-4777.	14.9	27
38	Quantum-Chemical Modeling of Energetic Materials. Advances in Quantum Chemistry, 2014, , 71-145.	0.8	24
39	Topography of Photochemical Initiation in Molecular Materials. Molecules, 2013, 18, 14148-14160.	3.8	22
40	Computational Design of Novel Energetic Materials: Dinitro-bis-triazolo-tetrazine. Journal of Physical Chemistry C, 2015, 119, 8512-8521.	3.1	21
41	Adsorption and decomposition of dimethyl methylphosphonate on size-selected (MoO₃)₃ clusters. Physical Chemistry Chemical Physics, 2018, 20, 4840-4850.	2.8	21
42	Energies of Electronic Transitions of Pentaerythritol Tetranitrate Molecules and Crystals. Journal of Physical Chemistry C, 2014, 118, 9324-9335.	3.1	20
43	Comprehensive End-to-End Design of Novel High Energy Density Materials: II. Computational Modeling and Predictions. Journal of Physical Chemistry C, 2017, 121, 23865-23874.	3.1	20
44	Room temperature decomposition of dimethyl methylphosphonate on cuprous oxide yields atomic phosphorus. Surface Science, 2019, 680, 75-87.	1.9	20
45	Dimethyl methylphosphonate adsorption and decomposition on MoO₂ as studied by ambient pressure x-ray photoelectron spectroscopy and DFT calculations. Journal of Physics Condensed Matter, 2018, 30, 134005.	1.8	19
46	Molecular Mechanisms of Shear Strain Sensitivity of the Energetic Crystals DADNE and TATB. Journal of Energetic Materials, 2010, 28, 66-77.	2.0	18
47	Defect states at organicâ€“inorganic interfaces: Insight from first principles calculations for pentaerythritol tetranitrate on MgO surface. Surface Science, 2015, 637-638, 19-28.	1.9	17
48	Electron Spectroscopy and Computational Studies of Dimethyl Methylphosphonate. Journal of Physical Chemistry A, 2016, 120, 1985-1991.	2.5	17
49	Modeling proton transfer and polarons in a molecular crystal diamino-dinitroethylene. Physical Review B, 2009, 80, .	3.2	16
50	Sarin Decomposition on Pristine and Hydroxylated ZnO: Quantum-Chemical Modeling. Journal of Physical Chemistry C, 2019, 123, 26432-26441.	3.1	16
51	Understanding Dimethyl Methylphosphonate Adsorption and Decomposition on Mesoporous CeO₂. ACS Applied Materials & Interfaces, 2021, 13, 54597-54609.	8.0	16
52	Degradation of Fatal Toxic Nerve Agents on Dry TiO₂. ACS Applied Materials & Interfaces, 2021, 13, 696-705.	8.0	15
53	Optical Absorption Energies of Molecular Defects in Pentaerythritol Tetranitrate Crystals: Quantum Chemical Modeling. Journal of Physical Chemistry C, 2014, 118, 26530-26542.	3.1	13
54	3-(4-Amino-1,2,5-oxadiazol-3-yl)-4-(4-nitro-1,2,5-oxadiazol-3-yl)-1,2,5-oxadiazole. MolBank, 2014, 2014, M824.	0.5	12

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55	Can a Photosensitive Oxide Catalyze Decomposition of Energetic Materials?. Journal of Physical Chemistry C, 2017, 121, 1153-1161.	3.1	12
56	First Principles Modeling of Oxygen Mobility in Perovskite SOFC Cathode and Oxygen Permeation Membrane Materials. ECS Transactions, 2011, 35, 823-830.	0.5	10
57	Photochemistry of the Î±-Al2O3-PETN Interface. Molecules, 2016, 21, 289.	3.8	8
58	Coupling Ambient Pressure X-ray Photoelectron Spectroscopy with Density Functional Theory to Study Complex Surface Chemistry and Catalysis. Topics in Catalysis, 2018, 61, 2175-2184.	2.8	8
59	Mechanisms of Degradation of Toxic Nerve Agents: Quantum-chemical Insight into Interactions of Sarin and Soman with Molybdenum Dioxide. Surface Science, 2020, 700, 121639.	1.9	7
60	The Structure and Decomposition Chemistry of Isomer Defects in a Crystalline DADNE. Journal of Energetic Materials, 2010, 28, 128-139.	2.0	6
61	Achieving tunable chemical reactivity through photo-initiation of energetic materials at metal oxide surfaces. Physical Chemistry Chemical Physics, 2020, 22, 25284-25296.	2.8	6
62	Modeling of shock compression of RDX with defects. AIP Conference Proceedings, 2000, , .	0.4	5
63	Role of Hydrogen Abstraction Reaction in Photocatalytic Decomposition of High Energy Density Materials. Journal of Physical Chemistry C, 2016, 120, 24835-24846.	3.1	5
64	NO2 Interactions with MoO3 and CuO at Atmospherically Relevant Pressures. Journal of Physical Chemistry C, 2021, 125, 16489-16497.	3.1	5
65	Recruiting Perovskites to Degrade Toxic Trinitrotoluene. Materials, 2021, 14, 7387.	2.9	5
66	The Use of Web-based Virtual X-Ray Diffraction Laboratory for Teaching Materials Science and Engineering. MRS Advances, 2017, 2, 1687-1692.	0.9	4
67	(Invited) The Effect of (La,Sr)MnO 3 Cathode Surface Termination on Its Electronic Structure. ECS Transactions, 2017, 77, 67-73.	0.5	2
68	Defect-Induced Decomposition of Energetic Nitro Compounds at MgO Surface. Surface Science, 2022, , 122085.	1.9	2
69	Titania Nanomaterials for Sarin Decomposition: Understanding Fundamentals. ACS Applied Nano Materials, 2022, 5, 6659-6670.	5.0	2
70	A computation of the frequency dependent dielectric function for energetic materials. AIP Conference Proceedings, 2000, , .	0.4	1
71	Electronic Excitations in Initiation of Chemistry in Molecular Solids. Materials Research Society Symposia Proceedings, 2001, 677, 241.	0.1	1
72	Effect of impurities on optical properties of pentaerythritol tetranitrate. , 2012, , .		1

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73	Searching for new energetic materials: Computational design of novel nitro-substituted heterocyclic explosives. AIP Conference Proceedings, 2017, , .	0.4	1
74	Manifestations of two-dimensional electron gas in molecular crystals. Surface Science, 2017, 657, 20-27.	1.9	1
75	Synthetic Alloys: Synthetic Crystals of Silver with Carbon: 3D Epitaxy of Carbon Nanostructures in the Silver Lattice (Adv. Funct. Mater. 30/2015). Advanced Functional Materials, 2015, 25, 4746-4746.	14.9	0
76	Achieving tunable sensitivity in composite high-energy density materials. AIP Conference Proceedings, 2017, , .	0.4	0