Quantum Chemical Strain Analysis For Mechanochemic

Accounts of Chemical Research
50, 1041-1048
DOI: 10.1021/acs.accounts.7b00038

Citation Report

#	Article	IF	Citations
1	Force-induced retro-click reaction of triazoles competes with adjacent single-bond rupture. Chemical Science, 2017, 8, 5567-5575.	7.4	20
2	An algorithm to locate optimal bond breaking points on a potential energy surface for applications in mechanochemistry and catalysis. Journal of Chemical Physics, 2017, 147, 152710.	3.0	22
3	Theoretical simulation of the infrared signature of mechanically stressed polymer solids. Beilstein Journal of Organic Chemistry, 2017, 13, 1710-1716.	2.2	6
5	Toward a theory of mechanochemistry: Simple models from the very beginnings. International Journal of Quantum Chemistry, 2018, 118, e25775.	2.0	18
6	Mechanochemistry of nucleosides, nucleotides and related materials. Beilstein Journal of Organic Chemistry, 2018, 14, 955-970.	2.2	68
7	Twist and Returnâ^'Induced Ring Strain Triggers Quick Relaxation of a (Z)-Stabilized Cyclobisazobenzene. Journal of Physical Chemistry Letters, 2018, 9, 4776-4781.	4.6	17
8	Mechanochemically Gated Photoswitching: Expanding the Scope of Polymer Mechanochromism. Synlett, 2019, 30, 1725-1732.	1.8	19
9	Ultrafast dynamics of highly constrained azobenzene macrocycles. EPJ Web of Conferences, 2019, 205, 09002.	0.3	0
10	Implementing the mechanical force into the conceptual DFT framework: understanding and predicting molecular mechanochemical properties. Physical Chemistry Chemical Physics, 2019, 21, 7378-7388.	2.8	25
11	Reaction milling for scalable synthesis of N, P-codoped covalent organic polymers for metal-free bifunctional electrocatalysts. Chemical Engineering Journal, 2019, 358, 427-434.	12.7	44
12	The hunt for reactive alkynes in bio-orthogonal click reactions: insights from mechanochemical and conceptual DFT calculations. Chemical Science, 2020, 11, 1431-1439.	7.4	21
13	A mechanochemical model for the simulation of molecules and molecular crystals under hydrostatic pressure. Journal of Chemical Physics, 2020, 153, 134503.	3.0	16
14	The Mechanism of Flexâ€Activation in Mechanophores Revealed By Quantum Chemistry. ChemPhysChem, 2020, 21, 2402-2406.	2.1	7
15	The rupture mechanism of rubredoxin is more complex than previously thought. Chemical Science, 2020, 11, 6036-6044.	7.4	1
16	Strain visualization for strained macrocycles. Chemical Science, 2020, 11, 3923-3930.	7.4	62
17	Tuning the Mechanical Properties of Metallopolymers via Ligand Interactions: A Combined Experimental and Theoretical Study. Macromolecules, 2020, 53, 2021-2030.	4.8	18
18	Quantum chemical modeling of molecules under pressure. International Journal of Quantum Chemistry, 2021, 121, e26208.	2.0	14
19	Mechanochemically Triggered Topology Changes in Expanded Porphyrins. Chemistry - A European Journal, 2021, 27, 3397-3406.	3.3	14

#	Article	IF	Citations
20	Modeling Molecules under Pressure with Gaussian Potentials. Journal of Chemical Theory and Computation, 2021, 17, 583-597.	5.3	17
21	The activation efficiency of mechanophores can be modulated by adjacent polymer composition. RSC Advances, 2021, 11, 7391-7396.	3.6	4
22	The many flavours of mechanochemistry and its plausible conceptual underpinnings. Nature Reviews Chemistry, 2021, 5, 148-167.	30.2	176
23	Mechanical degradation estimation of thermosets by peak shift assessment: General approach using infrared spectroscopy. Polymer, 2021, 221, 123585.	3.8	5
24	Designing Force Probes Based on Reversible 6Ï€-Electrocyclizations in Polyenes Using Quantum Chemical Calculations. Journal of Organic Chemistry, 2021, 86, 7477-7489.	3.2	5
25	Understanding the Mechanochemistry of Ladder-Type Cyclobutane Mechanophores by Single Molecule Force Spectroscopy. Journal of the American Chemical Society, 2021, 143, 12328-12334.	13.7	26
26	Stress-responsive properties of metallocenes in metallopolymers. Polymer Chemistry, 2021, 12, 2509-2521.	3.9	21
27	Harnessing the Power of Force: Development of Mechanophores for Molecular Release. Journal of the American Chemical Society, 2021, 143, 21461-21473.	13.7	54
29	Acid-free mechanochemical process to enhance the selective recycling of spent LiFePO4 batteries. Journal of Hazardous Materials, 2023, 443, 130160.	12.4	28
30	Outstanding Advantages, Current Drawbacks, and Significant Recent Developments in Mechanochemistry: A Perspective View. Crystals, 2023, 13, 124.	2.2	21
31	Effect of confinement and external mechanical force on the cleavage of the bond in a diatomic molecule. Molecular Physics, 0, , .	1.7	0
32	Theoretical understanding of mechanochemical (ball-milling) synthesis of thioethers: a CDFT approach. Journal of Mathematical Chemistry, 0, , .	1.5	1
33	Mechanochemical synthesis of organohalogen compounds: synthetic viewpoint. Russian Chemical Reviews, 2023, 92, .	6.5	0
34	Mechanochemical synthesis of halogenated heterocyclic compounds. Chemistry of Heterocyclic Compounds, 2023, 59, 525-533.	1.2	0
35	Wandering through quantum-mechanochemistry: from concepts to reactivity and switches. Physical Chemistry Chemical Physics, 0, , .	2.8	0