Debasis Sengupta

List of Publications by Year
in descending order

28	908	586496 16	591227 27
papers	citations	h-index	g-index

28	28	28	1177
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Anab initioBased Structure Property Relationship for Prediction of Ignition Delay of Hypergolic Ionic Liquids. Propellants, Explosives, Pyrotechnics, 2015, 40, 759-764.	1.0	14
2	Molecular Orbital Based Design Guideline for Hypergolic Ionic Liquids. Propellants, Explosives, Pyrotechnics, 2015, 40, 144-149.	1.0	15
3	High-Temperature Oxidation of SiC-Based Composite: Rate Constant Calculation from ReaxFF MD Simulations, Part II. Journal of Physical Chemistry C, 2013, 117, 5014-5027.	1.5	26
4	Oxidation of Silicon Carbide by O₂ and H₂O: A ReaxFF Reactive Molecular Dynamics Study, Part I. Journal of Physical Chemistry C, 2012, 116, 16111-16121.	1.5	177
5	Combined ab initio quantum chemistry and computational fluid dynamics calculations for prediction of gallium nitride growth. Journal of Crystal Growth, 2005, 279, 369-382.	0.7	74
6	A new approach to performing equilibrium surface reaction calculations and its application to predicting growth of gallium nitride. Journal of Crystal Growth, 2004, 261, 165-174.	0.7	5
7	Does the Ring Compound [(CH3)2GaNH2]3 Form During MOVPE of Gallium Nitride? Investigations via Density Functional and Reaction Rate Theories.. ChemInform, 2003, 34, no.	0.1	0
8	Does the Ring Compound [(CH3)2GaNH2]3Form during MOVPE of Gallium Nitride? Investigations via Density Functional and Reaction Rate Theories. Journal of Physical Chemistry B, 2003, 107, 291-297.	1.2	51
9	Unimolecular decomposition of the isomers of [HNO2]+ and [HNO2]â˜’ systems: a DFT study. Chemical Physics, 1999, 248, 147-159.	0.9	10
10	Rearrangement and Fragmentation Processes on the Potential Energy Surfaces of the (CHnS)+(n= 1â˜’4) Systems. Journal of Physical Chemistry A, 1999, 103, 772-778.	1.1	18
11	Theoretical analysis of reactions related to the HNO2 energy surface: OH + NO and H + NO2. Chemical Physics, 1998, 230, 1-11.	0.9	35
12	Theoretical Study of the H2+ NO and Related Reactions of [H2NO] Isomers. Journal of Physical Chemistry A, 1998, 102, 3175-3183.	1.1	57
13	Mechanism of NH2+CO2 formation in OH+HNCO reaction: Rate constant evaluation via ab initio calculations and statistical theory. Journal of Chemical Physics, 1997, 106, 9703-9707.	1.2	15
14	Regioselectivity of Oxetane Formation in the Photocycloaddition of Lowest3(n,Ï€*) State of Carbonyl Compounds:Â Interpretation Using Local Softness. Journal of Organic Chemistry, 1997, 62, 6404-6406.	1.7	37
15	Ab initio calculations and quantum statitiscal analysis of the SiH3+NO reaction. Chemical Physics Letters, 1997, 265, 35-40.	1.2	5
16	Reaction of Isocyanic Acid and Hydrogen Atom (H + HNCO):Â Theoretical Characterization. The Journal of Physical Chemistry, 1996, 100, 1615-1621.	2.9	42
17	Kinetic Analyses Combining Quantum Chemical and Quantum Statistical Methods:Â Some Case Studiesâ€. The Journal of Physical Chemistry, 1996, 100, 10956-10966.	2.9	19
18	Another Look at the Decomposition of Methyl Azide and Methanimine:Â How Is HCN Formed?. The Journal of Physical Chemistry, 1996, 100, 6499-6503.	2.9	62

#	Article	IF	Citations
19	Kinetic Study in a Microwave-Induced Plasma Afterglow of the Cu(2S) Atom Reaction with CH3Cl in the Temperature Range 389â^'853 K. The Journal of Physical Chemistry, 1996, 100, 8302-8307.	2.9	2
20	Ab initio calculation and kinetic analysis of the reaction of silylene with ethylene (SiH2 + C2H4). Molecular Physics, 1996, 89, 1567-1576.	0.8	23
21	A theoretical study of the reaction of SiH2 with C2H2 and C2D2. Chemical Physics Letters, 1995, 240, 513-520.	1.2	29
22	Can silacetylene be observed? A theoretical treatment of the tunneling effect. Chemical Physics Letters, 1995, 244, 83-88.	1.2	39
23	Further studies on Norrish type II reactions including a reaction in the first excited singlet state and cyclization of 1:4 biradicals. Journal of Photochemistry and Photobiology A: Chemistry, 1995, 86, 161-170.	2.0	6
24	Theoretical Study of the Thermal Decomposition of Acetic Acid: Decarboxylation Versus Dehydration. The Journal of Physical Chemistry, 1995, 99, 11883-11888.	2.9	93
25	Role of the HNO3â†”NOH Isomerization in reactions (i) NH(3Î£â^')+O(3P) and (ii) N(4S)+OH(2Î): Ab initio calculations and quantum statistical Riceâ€“Ramspergerâ€“Kassel analysis of the potential energy surfaces. Journal of Chemical Physics, 1994, 101, 3906-3915.	1.2	22
26	Role of tunneling of hydrogen in photoenolization of a ketone. International Journal of Quantum Chemistry, 1994, 52, 1317-1328.	1.0	9
27	Studies on the Norrish type II reactions of aliphatic Î±-diketones and the accompanying cyclization and disproportionation of 1:4 biradicals. Journal of Photochemistry and Photobiology A: Chemistry, 1993, 75, 151-162.	2.0	9
28	Role of barriers to conformational changes in ketones undergoing the Norrish type II process. Journal of Photochemistry and Photobiology A: Chemistry, 1991, 60, 149-159.	2.0	14