

Siddharth Dasgupta

List of Publications by Year in descending order

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34
papers

7,460
citations

236925

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377865

34
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34
all docs

34
docs citations

34
times ranked

6875
citing authors

#	ARTICLE	IF	CITATIONS
1	ReaxFF: A Reactive Force Field for Hydrocarbons. <i>Journal of Physical Chemistry A</i> , 2001, 105, 9396-9409.	2.5	4,490
2	Shock Waves in High-Energy Materials: The Initial Chemical Events in Nitramine RDX. <i>Physical Review Letters</i> , 2003, 91, 098301.	7.8	495
3	Carbon Cluster Formation during Thermal Decomposition of Octahydro-1,3,5,7-tetranitro-1,3,5,7-tetrazocine and 1,3,5-Triamino-2,4,6-trinitrobenzene High Explosives from ReaxFF Reactive Molecular Dynamics Simulations. <i>Journal of Physical Chemistry A</i> , 2009, 113, 10619-10640.	2.5	257
4	Hydrogen bonding in the benzene-ammonia dimer. <i>Nature</i> , 1993, 362, 735-737.	27.8	254
5	The Mechanism for Unimolecular Decomposition of RDX (1,3,5-Trinitro-1,3,5-triazine), an ab Initio Study. <i>Journal of Physical Chemistry A</i> , 2000, 104, 2261-2272.	2.5	241
6	Initiation Mechanisms and Kinetics of Pyrolysis and Combustion of JP-10 Hydrocarbon Jet Fuel. <i>Journal of Physical Chemistry A</i> , 2009, 113, 1740-1746.	2.5	213
7	Crystal Structures and Properties of Nylon Polymers from Theory. <i>Journal of the American Chemical Society</i> , 1996, 118, 12291-12301.	13.7	210
8	Mechanical properties and force field parameters for polyethylene crystal. <i>The Journal of Physical Chemistry</i> , 1991, 95, 2260-2272.	2.9	154
9	Mechanism for Unimolecular Decomposition of HMX (1,3,5,7-Tetranitro-1,3,5,7-tetrazocine), an ab Initio Study. <i>Journal of Physical Chemistry A</i> , 2001, 105, 1302-1314.	2.5	152
10	Distance Dependent Hydrogen Bond Potentials for Nucleic Acid Base Pairs from ab Initio Quantum Mechanical Calculations (LMP2/cc-pVTZ). <i>Journal of Physical Chemistry B</i> , 1997, 101, 4851-4859.	2.6	97
11	Molecular dynamics for very large systems on massively parallel computers: The MPSim program. <i>Journal of Computational Chemistry</i> , 1997, 18, 501-521.	3.3	80
12	Mechanism and Energetics for Complexation of ⁹⁰ Y with 1,4,7,10-Tetraazacyclododecane-1,4,7,10-tetraacetic Acid (DOTA), a Model for Cancer Radioimmunotherapy. <i>Journal of the American Chemical Society</i> , 1999, 121, 6142-6151.	13.7	73
13	Hessian-biased force fields from combining theory and experiment. <i>Journal of Chemical Physics</i> , 1989, 90, 7207-7215.	3.0	71
14	A detailed model for the decomposition of nitramines: RDX and HMX. <i>Journal of Computer-Aided Materials Design</i> , 2001, 8, 203-212.	0.7	69
15	Electron-transfer boat-vibration mechanism for superconductivity in organic molecules based on BEDT-TTF. <i>Journal of the American Chemical Society</i> , 1995, 117, 8154-8158.	13.7	66
16	Picosecond resonance Raman evidence for unrelaxed heme in the (carbonmonoxy)myoglobin photoproduct. <i>Biochemistry</i> , 1985, 24, 5295-5297.	2.5	49
17	Resonance Raman characterization of the 7-ns photoproduct of (carbonmonoxy)hemoglobin: implications for hemoglobin dynamics. <i>Biochemistry</i> , 1986, 25, 5941-5948.	2.5	49
18	Explanation of the Colossal Detonation Sensitivity of Silicon Pentaerythritol Tetranitrate (Si-PETN) Explosive. <i>Journal of the American Chemical Society</i> , 2009, 131, 7490-7491.	13.7	45

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19	The SAM Model for Wear Inhibitor Performance of Dithiophosphates on Iron Oxide. Journal of Physical Chemistry B, 1997, 101, 7702-7709.	2.6	44
20	Structures, Vibrations, and Force Fields of Dithiophosphate Wear Inhibitors from ab Initio Quantum Chemistry. The Journal of Physical Chemistry, 1996, 100, 15760-15769.	2.9	43
21	The Hessian biased singular value decomposition method for optimization and analysis of force fields. Journal of Chemical Physics, 1996, 104, 2898-2920.	3.0	39
22	Chromophore-in-Protein Modeling of the Structures and Resonance Raman Spectra for Type 1 Copper Proteins. Journal of the American Chemical Society, 1998, 120, 12791-12797.	13.7	37
23	Strategies for multiscale modeling and simulation of organic materials: polymers and biopolymers. Computational and Theoretical Polymer Science, 2001, 11, 329-343.	1.1	36
24	Ultraviolet resonance Raman spectra of hemoglobin excited at 200 and 218 nm: tertiary and quaternary structure differences. Journal of the American Chemical Society, 1985, 107, 3370-3371.	13.7	29
25	MSX Force Field and Vibrational Frequencies for BEDT-TTF (Neutral and Cation). Journal of Physical Chemistry A, 1997, 101, 1975-1981.	2.5	29
26	Polyoxymethylene: the Hessian biased force field for molecular dynamics simulations. The Journal of Physical Chemistry, 1993, 97, 10891-10902.	2.9	25
27	Stabilizing the Boat Conformation of Cyclohexane Rings. Journal of the American Chemical Society, 1995, 117, 6532-6534.	13.7	25
28	The Role of Water Near Cytochrome a in Cytochrome c Oxidase. Annals of the New York Academy of Sciences, 1988, 550, 223-237.	3.8	23
29	Ab initio derived spectroscopic quality force fields for molecular modeling and dynamics. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 1997, 53, 1347-1363.	3.9	16
30	Hessian biased force field for polysilane polymers. The Journal of Physical Chemistry, 1995, 99, 13321-13333.	2.9	13
31	Theoretical studies on VPI-5. 3.. Computational Materials Science, 1999, 14, 135-137.	3.0	11
32	Thermal Decomposition of Energetic Materials by ReaxFF Reactive Molecular Dynamics. AIP Conference Proceedings, 2006, , .	0.4	11
33	Transient resonance Raman spectroscopy shows unrelaxed heme following CO photodissociation from cytochrome-c peroxidase. BBA - Proteins and Proteomics, 1986, 873, 88-91.	2.1	9
34	Resonance Raman spectroscopic evidence that carp deoxyhemoglobin remains in a T-like quaternary structure at high pH: implications for cooperativity. Biochemistry, 1986, 25, 1940-1944.	2.5	5