Siddharth Dasgupta

List of Publications by Year
in descending order

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34 papers	7,460 citations	270111 25 h-index	425179 34 g-index
34 all docs	34 docs citations	34 times ranked	7923 citing authors

#	Article	IF	Citations
1	Explanation of the Colossal Detonation Sensitivity of Silicon Pentaerythritol Tetranitrate (Si-PETN) Explosive. Journal of the American Chemical Society, 2009, 131, 7490-7491.	6.6	45
2	Initiation Mechanisms and Kinetics of Pyrolysis and Combustion of JP-10 Hydrocarbon Jet Fuel. Journal of Physical Chemistry A, 2009, 113, 1740-1746.	1.1	213
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. Journal of Physical Chemistry A, 2009, 113, 10619-10640.	1.1	257
4	Thermal Decomposition of Energetic Materials by ReaxFF Reactive Molecular Dynamics. AIP Conference Proceedings, 2006, , .	0.3	11
5	Shock Waves in High-Energy Materials: The Initial Chemical Events in Nitramine RDX. Physical Review Letters, 2003, 91, 098301.	2.9	495
6	Mechanism for Unimolecular Decomposition of HMX (1,3,5,7-Tetranitro-1,3,5,7-tetrazocine), an ab Initio Study. Journal of Physical Chemistry A, 2001, 105, 1302-1314.	1.1	152
7	ReaxFF:Â A Reactive Force Field for Hydrocarbons. Journal of Physical Chemistry A, 2001, 105, 9396-9409.	1.1	4,490
8	Strategies for multiscale modeling and simulation of organic materials: polymers and biopolymers. Computational and Theoretical Polymer Science, 2001, 11, 329-343.	1.1	36
9	A detailed model for the decomposition of nitramines: RDX and HMX. Journal of Computer-Aided Materials Design, 2001, 8, 203-212.	0.7	69
10	The Mechanism for Unimolecular Decomposition of RDX (1,3,5-Trinitro-1,3,5-triazine), an ab Initio Study. Journal of Physical Chemistry A, 2000, 104, 2261-2272.	1.1	241
11	Theoretical studies on VPI-5. 3.. Computational Materials Science, 1999, 14, 135-137.	1.4	11
12	Mechanism and Energetics for Complexation of90Y with 1,4,7,10-Tetraazacyclododecane-1,4,7,10-tetraacetic Acid (DOTA), a Model for Cancer Radioimmunotherapy. Journal of the American Chemical Society, 1999, 121, 6142-6151.	6.6	73
13	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.	6.6	37
14	MSX Force Field and Vibrational Frequencies for BEDT-TTF (Neutral and Cation). Journal of Physical Chemistry A, 1997, 101, 1975-1981.	1.1	29
15	The SAM Model for Wear Inhibitor Performance of Dithiophosphates on Iron Oxide. Journal of Physical Chemistry B, 1997, 101, 7702-7709.	1.2	44
16	Distance Dependent Hydrogen Bond Potentials for Nucleic Acid Base Pairs from ab Initio Quantum Mechanical Calculations (LMP2/cc-pVTZ). Journal of Physical Chemistry B, 1997, 101, 4851-4859.	1.2	97
17	Ab initio derived spectroscopic quality force fields for molecular modeling and dynamics. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 1997, 53, 1347-1363.	2.0	16
18	Molecular dynamics for very large systems on massively parallel computers: The MPSim program. Journal of Computational Chemistry, 1997, 18, 501-521.	1.5	80

#	Article	IF	Citations
19	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
20	Crystal Structures and Properties of Nylon Polymers from Theory. Journal of the American Chemical Society, 1996, 118, 12291-12301.	6.6	210
21	The Hessian biased singular value decomposition method for optimization and analysis of force fields. Journal of Chemical Physics, 1996, 104, 2898-2920.	1.2	39
22	Hessian biased force field for polysilane polymers. The Journal of Physical Chemistry, 1995, 99, 13321-13333.	2.9	13
23	Electron-transfer boat-vibration mechanism for superconductivity in organic molecules based on BEDT-TTF. Journal of the American Chemical Society, 1995, 117, 8154-8158.	6.6	66
24	Stabilizing the Boat Conformation of Cyclohexane Rings. Journal of the American Chemical Society, 1995, 117, 6532-6534.	6.6	25
25	Hydrogen bonding in the benzeneâ€“ammonia dimer. Nature, 1993, 362, 735-737.	13.7	254
26	Polyoxymethylene: the Hessian biased force field for molecular dynamics simulations. The Journal of Physical Chemistry, 1993, 97, 10891-10902.	2.9	25
27	Mechanical properties and force field parameters for polyethylene crystal. The Journal of Physical Chemistry, 1991, 95, 2260-2272.	2.9	154
28	Hessianâ€biased force fields from combining theory and experiment. Journal of Chemical Physics, 1989, 90, 7207-7215.	1.2	71
29	The Role of Water Near Cytochrome a in Cytochrome c Oxidase. Annals of the New York Academy of Sciences, 1988, 550, 223-237.	1.8	23
30	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.	1.2	5
31	Resonance Raman characterization of the 7-ns photoproduct of (carbonmonoxy)hemoglobin: implications for hemoglobin dynamics. Biochemistry, 1986, 25, 5941-5948.	1.2	49
32	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
33	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.	6.6	29
34	Picosecond resonance Raman evidence for unrelaxed heme in the (carbonmonoxy)myoglobin photoproduct. Biochemistry, 1985, 24, 5295-5297.	1.2	49