

Mustafa BÃ-yÃœkata

List of Publications by Year in descending order

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129
citing authors

#	ARTICLE	IF	CITATIONS
1	Density functional study of Al _n clusters for n=1–14. Journal of Alloys and Compounds, 2011, 509, 4214-4234.	5.5	34
2	An investigation of hydrogen bonded neutral B ₄ H _n (n=1–11) and anionic clusters: Density functional study. Computational and Theoretical Chemistry, 2007, 805, 91-100.	1.5	23
3	REACTION DYNAMICS OF Ni _n (n =19 and 20) WITH D ₂ : DEPENDENCE ON CLUSTER SIZE, TEMPERATURE AND INITIAL ROVIBRATIONAL STATES OF THE MOLECULE. International Journal of Modern Physics C, 2005, 16, 295-308.	1.7	18
4	DFT study of Al doped cage B ₁₂ H _n clusters. International Journal of Hydrogen Energy, 2011, 36, 8392-8402.	7.1	11
5	Reactions of small Ni clusters with a diatomic molecule: MD simulation of D ₂ +Ni _n (n=7–10) systems. Surface Science, 2000, 454-456, 310-315.	1.9	10
6	Conformational and vibrational analysis of 2-, 3- and 4-trifluoromethylbenzaldehyde by ab initio Hartree-Fock, density functional theory and Moller-Plesset perturbation theory calculations. Computational and Theoretical Chemistry, 2008, 861, 122-130.	1.5	9
7	MD study of energetics, melting and isomerization of aluminum microclusters. Brazilian Journal of Physics, 2006, 36, 720-724.	1.4	8
8	Molecule-surface interaction: dissociative chemisorption of a D ₂ (v=0, j=0) molecule on rigid low index Ni surfaces. Surface Science, 2004, 562, 183-194.	1.9	7
9	Molecular-dynamics study of possible packing sequence of medium size gold clusters: Au ₂ –Au ₄₃ . Physica E: Low-Dimensional Systems and Nanostructures, 2006, 33, 182-190.	2.7	5
10	Dissociative Chemisorption of an H ₂ (v, j) Molecule on Rigid Ni (100) Surface: Dependence on Surface Topologies and Initial Rovibrational States of the Molecules. Chinese Physics Letters, 2005, 22, 420-423.	3.3	2
11	MOLECULAR DYNAMICS STUDY OF Tin, Van AND Chromium CLUSTERS. Journal of Theoretical and Computational Chemistry, 2007, 06, 81-97.	1.8	2
12	Ab Initio Hartree-Fock and Density Functional Theory Study on Molecular Structures, Energies, and Vibrational Frequencies of 2-Amino-3-, 4-, and 5-Nitropyridine. Zeitschrift Fur Naturforschung - Section A Journal of Physical Sciences, 2010, 65, 107-112.	1.5	2
13	Synthesis and DFT study of Cd(II) and Hg(II) complexes of ONNO-type Schiff bases. Inorganic and Nano-Metal Chemistry, 2017, 47, 850-858.	1.6	1
14	Effects of molecular rovibrational states and surface topologies for molecule-surface interaction: chemisorption dynamics of D ₂ collision with rigid Ni surfaces. Brazilian Journal of Physics, 2006, 36, 725-729.	1.4	1
15	Hartree-Fock and Density Functional Theory analysis of N-phenyl-1,2-naphthylamine. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2013, 114, 377-393.	3.9	0