

Murat Atis

List of Publications by Year in descending order

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#	ARTICLE	IF	CITATIONS
1	Determination of Complete Melting and Surface Premelting Points of Silver Nanoparticles by Molecular Dynamics Simulation. <i>Journal of Physical Chemistry C</i> , 2013, 117, 12289-12298.	3.1	97
2	Some characteristic behavior of spin-1 Ising nanotube. <i>Physics Letters, Section A: General, Atomic and Solid State Physics</i> , 2011, 375, 3547-3551.	2.1	63
3	Structure and energetic of B _n (n = 2–12) clusters: Electronic structure calculations. <i>International Journal of Quantum Chemistry</i> , 2007, 107, 729-744.	2.0	50
4	Molecular Dynamics Simulation of Sintering and Surface Premelting of Silver Nanoparticles. <i>Materials Transactions</i> , 2013, 54, 884-889.	1.2	49
5	Structural, spectral, optical and antimicrobial properties of synthesized 1-benzoyl-3-furan-2-ylmethyl-thiourea. <i>Journal of Molecular Structure</i> , 2013, 1048, 69-77.	3.6	39
6	Half-Metallic Ferrimagnetism in the Mn ₂ NbAl Full-Heusler Compound: a First-Principles Study. <i>Journal of Superconductivity and Novel Magnetism</i> , 2016, 29, 187-192.	1.8	34
7	Structural, antimicrobial and computational characterization of 1-benzoyl-3-(5-chloro-2-hydroxyphenyl)thiourea. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2012, 98, 290-301.	3.9	31
8	Half-metallicity in the inverse Heusler Ti ₂ RuSn alloy: A first-principles prediction. <i>Journal of Magnetism and Magnetic Materials</i> , 2017, 426, 473-478.	2.3	27
9	Boron-doped hydrogenated Al ₃ clusters: A material for hydrogen storage. <i>Journal of Alloys and Compounds</i> , 2016, 667, 275-281.	5.5	26
10	Density Functional Study of Physical and Chemical Properties of Nano Size Boron Clusters: B _{<sub>n</sub>} (_{i>n</i>= 1320). <i>Chinese Journal of Chemical Physics</i>, 2009, 22, 380-388.}	1.3	23
11	Magnetism and Half-Metallicity in the Fe ₂ ZrP Heusler Alloy. <i>Journal of Superconductivity and Novel Magnetism</i> , 2016, 29, 2573-2578.	1.8	20
12	Molecular dynamics simulation of melting behaviour of small gold clusters: AuN _{<sub>n</sub>} (N=12–14). <i>Physica Scripta</i> , 2007, 75, 111-118.	2.5	17
13	STRUCTURE AND DYNAMICAL PROPERTIES OF AuN, N = 12–14 CLUSTERS: MOLECULAR DYNAMICS SIMULATION. <i>International Journal of Modern Physics C</i> , 2005, 16, 99-116.	1.7	11
14	Structures and melting of AgN(N= 7, 12–14) clusters. <i>Modelling and Simulation in Materials Science and Engineering</i> , 2005, 13, 1411-1432.	2.0	10
15	Ab initio search for global minimum structures of neutral and anionic hydrogenated Li ₅ clusters. <i>Chemical Physics</i> , 2013, 418, 14-21.	1.9	9
16	Search for the global minimum structures of AlB _{<sub>3</sub>} H _{<sub>2</sub>} _{<sub>i</sub>} _{<sub>n</sub>} _{<sub>i</sub>} (_{i>n</i>= 0–6) clusters. <i>Journal of Computational Chemistry</i>, 2015, 36, 385-391.}	3.0	19
17	Structural transformations in the carborane series: C _{<sub>n</sub>} B ₆ H _{<sub>6</sub>} (n= 0–6) upon substitution of boron by carbon. <i>Inorganica Chimica Acta</i> , 2016, 453, 626-632.	2.4	7
18	New organocobaloxime derivatives – Synthesis, characterization, catalase-like activity and DFT studies. <i>Journal of Organometallic Chemistry</i> , 2014, 756, 10-18.	1.8	6

#	ARTICLE	IF	CITATIONS
19	PARALLELIZATION OF A MOLECULAR DYNAMICS SIMULATION OF AN ION-SURFACE COLLISION SYSTEM: Ar–Ni(100). International Journal of Modern Physics C, 2005, 16, 969-990.	1.7	4
20	Stochastic search, fragmentation, electronic and reactivity properties of neutral and cationic hydrogenated Li ₆ clusters. Journal of Molecular Structure, 2014, 1065-1066, 65-73.	3.6	4
21	Structure, Ionization, and Fragmentation of Hydrogenated Aluminoboron Clusters: Al ₂ B ₂ H _{2n} (n=0–6). ChemistrySelect, 2016, 1, 3804-3811.	1.5	3
22	Structural and computational characterization of 4 ² ,4 ² ,6 ² ,6 ² -tetrachloro-3-(2-methoxyethyl)-3H,4H-spiro-1,3,2-benzoxaza phosphinine-2,2 ² -[1,3,5,2,4,6]6 triazatriphosphinine. Journal of Molecular Structure, 2016, 1117, 276-282.	3	
23	Surface modification by 1 keV ion impact: molecular dynamics study of an Ar–Ni(100) collision system. Modelling and Simulation in Materials Science and Engineering, 2008, 16, 035003.	2.0	1