

Åakir Erko Å

List of Publications by Year in descending order

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84

times ranked

867

citing authors

#	ARTICLE	IF	CITATIONS
1	Empirical many-body potential energy functions used in computer simulations of condensed matter properties. <i>Physics Reports</i> , 1997, 278, 79-105.	25.6	118
2	Structural and electronic properties of single-wall ZnO nanotubes. <i>Physica E: Low-Dimensional Systems and Nanostructures</i> , 2005, 28, 162-170.	2.7	56
3	AM1 treatment of endohedrally hydrogen doped fullerene, nH ₂ @C ₆₀ . <i>Computational and Theoretical Chemistry</i> , 2003, 638, 37-40.	1.5	52
4	Monte Carlo computer simulation of copper clusters. <i>Physical Review A</i> , 1999, 60, 3053-3057.	2.5	48
5	Theoretical investigation of quercetin and its radical isomers. <i>Computational and Theoretical Chemistry</i> , 2003, 631, 141-146.	1.5	47
6	Stability of gold clusters: molecular-dynamics simulations. <i>Physica E: Low-Dimensional Systems and Nanostructures</i> , 2000, 8, 210-218.	2.7	44
7	Analyzing Fe-Zn system using molecular dynamics, evolutionary neural nets and multi-objective genetic algorithms. <i>Computational Materials Science</i> , 2009, 46, 821-827.	3.0	42
8	Structural and electronic properties of AlkTilNimmicroclusters: Density-functional-theory calculations. <i>Physical Review A</i> , 2002, 66, .	2.5	29
9	Ammonia deposition in fullerene: (NH ₃) _n @C ₆₀ . <i>Computational and Theoretical Chemistry</i> , 2003, 640, 57-61.	1.5	28
10	Molecular-dynamics simulations of silver clusters. <i>Physica E: Low-Dimensional Systems and Nanostructures</i> , 1999, 5, 1-6.	2.7	27
11	EMPIRICAL POTENTIAL ENERGY FUNCTIONS USED IN THE SIMULATIONS OF MATERIALS PROPERTIES. , 2001, , 1-103.		27
12	AlTiNi Ternary Alloy Clusters: Molecular Dynamics Simulations and Density Functional Theory Calculations. <i>Journal of Physical Chemistry B</i> , 2003, 107, 12118-12125.	2.6	26
13	Energetics and structural stability of lanthanum microclusters. <i>Chemical Physics Letters</i> , 1999, 314, 203-209.	2.6	21
14	Genetic Algorithms in Application to the Geometry Optimization of Nanoparticles. <i>Algorithms</i> , 2009, 2, 410-428.	2.1	20
15	Development of the ReaxFF Reactive Force Field for Inherent Point Defects in the Si/Silica System. <i>Journal of Physical Chemistry A</i> , 2019, 123, 4303-4313.	2.5	20
16	Comment on Modelling complexes of H ₂ molecules in fullerenes by H. Dodziuk [Chem. Phys. Lett. 410 (2005) 39]. <i>Chemical Physics Letters</i> , 2006, 426, 222-223.	2.6	17
17	Application of Genetic Algorithms to Geometry Optimization of Microclusters: A Comparative Study of Empirical Potential Energy Functions for Silicon. <i>Materials and Manufacturing Processes</i> , 2003, 18, 329-339.	4.7	16
18	STRUCTURAL AND ELECTRONIC PROPERTIES OF CARBON NANOTUBES. <i>International Journal of Modern Physics C</i> , 2000, 11, 175-182.	1.7	15

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19	FROM CARBON NANOTUBES TO CARBON NANORODS. International Journal of Modern Physics C, 2000, 11, 1247-1255.	1.7	14
20	STRUCTURAL PROPERTIES OF CARBON NANORODS: MOLECULAR-DYNAMICS SIMULATIONS. International Journal of Modern Physics C, 2002, 13, 367-373.	1.7	14
21	Stability of Carbon Nanoion C ₂₀ @C ₆₀ @C ₂₄₀ : Molecular Dynamics Simulations. Nano Letters, 2002, 2, 215-217.	9.1	13
22	Structural features and energetics of Zn _n -Cd _m (n=7,8) microclusters and Zn ₅₀ -Cd ₅₀ , and Zn ₂₅ Cd ₂₅ nanoparticles: Molecular-dynamics simulations. Physical Review A, 2003, 68, .	2.5	12
23	EFFECT OF CHIRALITY ON THE STABILITY OF CARBON NANOTUBES: MOLECULAR-DYNAMICS SIMULATIONS. International Journal of Modern Physics C, 2001, 12, 865-870.	1.7	11
24	Theoretical investigation of flavonoids naringenin and genistein. Computational and Theoretical Chemistry, 2002, 583, 163-167.	1.5	11
25	Structural properties of defected ZnO nanoribbons under uniaxial strain: Molecular dynamics simulations. Current Applied Physics, 2014, 14, 57-67.	2.4	11
26	Development of a ReaxFF Reactive Force Field for Interstitial Oxygen in Germanium and Its Application to GeO ₂ /Ge Interfaces. Journal of Physical Chemistry C, 2019, 123, 1208-1218.	3.1	11
27	Genetic Algorithm Application to the Structural Properties of Si-Ge Mixed Clusters. Materials and Manufacturing Processes, 2009, 24, 250-254.	4.7	10

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37	Molecular-dynamics simulations of silicene nanoribbons under strain. <i>Physica Status Solidi (B): Basic Research</i> , 2012, 249, 74-81.	1.5	7
38	EMPIRICAL MANY-BODY POTENTIAL ENERGY FUNCTION CALCULATION FOR LITHIUM CLUSTERS IN BCC AND FCC SURFACE SYMMETRIES, AND CHEMISORPTION ENERGY OF ATOMIC OXYGEN ON LITHIUM BCC CLUSTERS. <i>Modern Physics Letters A</i> , 1995, 10, 125-131.	1.2	6
39	MOLECULAR-DYNAMICS SIMULATIONS OF NICKEL CLUSTERS. <i>International Journal of Modern Physics C</i> , 2000, 11, 1013-1024.	1.7	6
40	AN ALGORITHM TO GENERATE TOROIDAL AND HELICAL CAGE STRUCTURES USING PENTAGONS, HEXAGONS AND HEPTAGONS. <i>International Journal of Modern Physics C</i> , 2004, 15, 267-278.	1.7	6
41	Molecular-dynamics simulations of surface and bulk properties of Zn, Cd, and ZnCd systems. <i>Physica Status Solidi (B): Basic Research</i> , 2004, 241, 292-297.	1.5	6
42	STRUCTURAL AND ELECTRONIC PROPERTIES OF c-BN(110) SURFACE AND SURFACE POINT DEFECTS. <i>International Journal of Modern Physics C</i> , 2006, 17, 795-803.	1.7	6
43	THE EFFECT OF PBC ON THE SIMULATION OF NANOTUBES. <i>International Journal of Modern Physics C</i> , 2000, 11, 547-551.	1.7	5
44	Structural and electronic properties of xanthohumol metabolite. <i>Computational and Theoretical Chemistry</i> , 2002, 583, 169-172.	1.5	5
45	Theoretical investigation of sulforaphane molecule. <i>Computational and Theoretical Chemistry</i> , 2005, 714, 81-85.	1.5	5
46	STRUCTURAL, ELECTRONIC AND QSAR PROPERTIES OF THE CYFLUTHRIN MOLECULE: A THEORETICAL AM1 AND PM3 TREATMENT. <i>International Journal of Modern Physics C</i> , 2006, 17, 1391-1402.	1.7	5
47	ENERGETICS OF ARSENIC TERMINATED GaAs(001) SURFACES. <i>International Journal of Modern Physics C</i> , 2000, 11, 1225-1237.	1.7	4
48	Molecular-dynamics simulations of gold clusters. <i>Advances in Quantum Chemistry</i> , 2000, , 353-364.	0.8	4
49	ENERGETICS AND STABILITY OF DISCRETE CHARGE DISTRIBUTION ON THE SURFACE OF A SPHERE. <i>International Journal of Modern Physics C</i> , 2001, 12, 293-305.	1.7	4
50	MOLECULAR-DYNAMICS SIMULATIONS OF CARBON NANOCAGE STRUCTURES: NANOBALLS AND NANOTOROIDS. <i>International Journal of Modern Physics C</i> , 2001, 12, 685-690.	1.7	4
51	DECOMPOSITION OF SiH4 ON THE SA TYPE STEPPED Si(100) SURFACE. <i>Surface Review and Letters</i> , 2002, 09, 1401-1407.	1.1	4
52	STRUCTURAL AND ELECTRONIC PROPERTIES OF MAGNESIUM DIBORIDE. <i>International Journal of Modern Physics C</i> , 2003, 14, 483-489.	1.7	4
53	JUNCTION FORMATION IN CROSSED NANOTUBES UNDER PRESSURE: MOLECULAR-DYNAMICS SIMULATIONS. <i>International Journal of Modern Physics C</i> , 2005, 16, 1371-1377.	1.7	4
54	GOLD DEPOSITION ON GaAs(001) SURFACES: MOLECULAR-DYNAMICS SIMULATIONS. <i>International Journal of Modern Physics C</i> , 2002, 13, 759-769.	1.7	3

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55	Quantum chemical investigation of nitrotyrosine (3-nitro-l-tyrosine) and 8-nitroguanine. <i>Amino Acids</i> , 2010, 38, 319-327.	2.7	3
56	STRUCTURAL AND ELECTRONIC PROPERTIES OF CARBON NANOBALLS: C20, C60, AND C20@C60. <i>International Journal of Modern Physics C</i> , 2001, 12, 1391-1399.	1.7	2
57	ELECTRONIC BAND STRUCTURE OF STEPPED Si(100) SURFACES. <i>Surface Review and Letters</i> , 2001, 08, 61-66.	1.1	2
58	SIMULATION OF THE CASIMIRâ€“POLDER EFFECT FOR VARIOUS GEOMETRIES. <i>International Journal of Modern Physics C</i> , 2002, 13, 979-985.	1.7	2
59	STRUCTURAL AND ELECTRONIC PROPERTIES OF AlP DOPED HÄœCKEL TYPE CYCLACENE WITH FOUR BENZENOID RINGS. <i>International Journal of Modern Physics C</i> , 2003, 14, 1183-1189.	1.7	2
60	A COMPARATIVE STUDY OF EMPIRICAL POTENTIAL ENERGY FUNCTIONS: APPLICATIONS TO SILICON MICROCLUSTERS. <i>International Journal of Modern Physics C</i> , 2004, 15, 403-408.	1.7	2
61	METAL ATOM ENDOHEDRALLY DOPED C20 CAGE STRUCTURE: (X@C20; X =Ni, Fe, Co). <i>International Journal of Modern Physics C</i> , 2005, 16, 1553-1560.	1.7	2
62	STRUCTURAL PROPERTIES OF COPPER NANOPARTICLES: MODIFIED DIFFUSION MONTE CARLO SIMULATIONS. <i>International Journal of Modern Physics C</i> , 2006, 17, 1171-1177.	1.7	2
63	SINGLE WALL BAMBOO SHAPED CARBON NANOTUBE: A MOLECULAR DYNAMICS AND ELECTRONIC STUDY. <i>International Journal of Modern Physics C</i> , 2006, 17, 187-196.	1.7	2
64	Quantumâ€chemical treatment of the linoleic acid molecule and two of its conjugated isomers. <i>European Journal of Lipid Science and Technology</i> , 2009, 111, 1035-1041.	1.5	2
65	DECOMPOSITION OF C60 MOLECULES ON Si(100)(2 Å– 1) SURFACE. <i>International Journal of Modern Physics C</i> , 2000, 11, 1067-1076.	1.7	1
66	MOLECULAR-DYNAMICS SIMULATION OF STEPPED Si(100) SURFACE. <i>International Journal of Modern Physics C</i> , 2000, 11, 999-1011.	1.7	1
67	MOLECULAR-DYNAMICS SIMULATION OF RADIATION DAMAGE ON COPPER CLUSTERS. <i>International Journal of Modern Physics C</i> , 2000, 11, 1025-1032.	1.7	1
68	ADSORPTION OF HYDROGEN AND OXYGEN ON SINGLE AND DOUBLE LAYER STEPPED SI(100) SURFACES. <i>International Journal of Modern Physics B</i> , 2001, 15, 2261-2274.	2.0	1
69	Cluster, Surface and Bulk Properties of ZnCd Binary Alloys: Molecular-Dynamics Simulations. <i>Materials Science Forum</i> , 2005, 502, 51-56.	0.3	1
70	THERMAL STABILITY OF BENZOROD ARRAYS: MOLECULAR-DYNAMICS SIMULATIONS. <i>International Journal of Modern Physics C</i> , 2005, 16, 827-834.	1.7	1
71	STRUCTURAL AND ELECTRONIC PROPERTIES OF (C _n Li) ⁺ CLUSTER IONS. <i>International Journal of Modern Physics C</i> , 2005, 16, 271-280.	1.7	1
72	STRUCTURAL AND ELECTRONIC PROPERTIES OF THE DPPC MOLECULE. <i>International Journal of Modern Physics C</i> , 2006, 17, 967-974.	1.7	1

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73	STRUCTURAL AND ELECTRONIC PROPERTIES OF DIPROPYL SULFIDE: A THEORETICAL INVESTIGATION. International Journal of Modern Physics C, 2006, 17, 1179-1190.	1.7	1
74	Structural Properties of Carbon Nanogears. Fullerenes Nanotubes and Carbon Nanostructures, 2008, 16, 30-39.	2.1	1
75	Modeling of Nanostructures., 2015,, 1-55.		1
76	GENERAL ANALYTIC DENSITY DISTRIBUTION FUNCTION FOR ATOMS. International Journal of Modern Physics C, 2000, 11, 1167-1177.	1.7	0
77	ADSORPTION OF WATER ON SINGLE AND DOUBLE LAYER STEPPED Si(100) SURFACES. Surface Review and Letters, 2001, 08, 251-259.	1.1	0
78	OPTICAL TRANSITIONS IN A PARABOLIC GaAs/Ga _{1-x} Al _x As SUPERLATTICES. Surface Review and Letters, 2001, 08, 321-325.	1.1	0
79	IMPACT OF GEOMETRY ON THE HYDROGEN STORAGE PROPERTIES OF TITANIUM CARBIDE: A DFT STUDY ON THE MODEL <chem>TiC</chem><sub>4</sub><chem>H</chem><sub>4</sub>. International Journal of Modern Physics C, 2007, 18, 1951-1960.</chem>	1.7	0
80	Monte Carlo geometry optimization of Si _n ($n \approx 1/2$ 71) clusters. Journal of Computational Methods in Sciences and Engineering, 2008, 7, 233-240.	0.2	0
81	Structural properties of lithium clusters: A Monte Carlo application. Journal of Computational Methods in Sciences and Engineering, 2008, 7, 409-416.	0.2	0
82	Modeling of Nanostructures., 2012,, 995-1041.		0
83	Modeling of Nanostructures., 2017,, 1459-1513.		0
84	Nanoassemblies of Porphyrin Derivatives. , 2022,, 1-38.		0