Åakir ErkoÃ§

List of Publications by Year
in descending order

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84	957	516710 16	501196 28
papers	citations	h-index	g-index

84	84	84	867
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Nanoassemblies of Porphyrin Derivatives. , 2022, , 1-38.		0
2	Development of the ReaxFF Reactive Force Field for Inherent Point Defects in the Si/Silica System. Journal of Physical Chemistry A, 2019, 123, 4303-4313.	2.5	20
3	Development of a ReaxFF Reactive Force Field for Interstitial Oxygen in Germanium and Its Application to GeO2/Ge Interfaces. Journal of Physical Chemistry C, 2019, 123, 1208-1218.	3.1	11
4	Modeling of Nanostructures. , 2017, , 1459-1513.		0
5	Study of the Influence of Transition Metal Atoms on Electronic and Magnetic Properties of Graphyne Nanotubes Using Density Functional Theory. Fullerenes Nanotubes and Carbon Nanostructures, 2015, 23, 494-499.	2.1	8
6	Modeling of Nanostructures. , 2015, , 1-55.		1
7	Structural properties of defected ZnO nanoribbons under uniaxial strain: Molecular dynamics simulations. Current Applied Physics, 2014, 14, 57-67.	2.4	11
8	GROUP 12 ELEMENTS AND THEIR SMALL CLUSTERS: ELECTRIC DIPOLE POLARIZABILITY OFZn,CdANDHg,Zn₂DIMER AND HIGHERZn_nMICROCLUSTERS AND NEUTRAL, CATIONIC AND ANIONIC ZINC OXIDE MOLECULES (ZnO,ZnO⁺ANDZnO⁻). International Journal of Modern Physics B, 2012, 26, 1230003.	2.0	8
9	Molecularâ€dynamics simulations of silicene nanoribbons under strain. Physica Status Solidi (B): Basic Research, 2012, 249, 74-81.	1.5	7
10	Modeling of Nanostructures. , 2012, , 995-1041.		0
11	Quantum chemical investigation of nitrotyrosine (3-nitro-l-tyrosine) and 8-nitroguanine. Amino Acids, 2010, 38, 319-327.	2.7	3
12	Genetic Algorithms in Application to the Geometry Optimization of Nanoparticles. Algorithms, 2009, 2, 410-428.	2.1	20
13	Genetic Algorithm Application to the Structural Properties of Siâ€“Ge Mixed Clusters. Materials and Manufacturing Processes, 2009, 24, 250-254.	4.7	10
14	Quantumâ€chemical treatment of the linoleic acid molecule and two of its conjugated isomers. European Journal of Lipid Science and Technology, 2009, 111, 1035-1041.	1.5	2
15	Analyzing Feâ€“Zn system using molecular dynamics, evolutionary neural nets and multi-objective genetic algorithms. Computational Materials Science, 2009, 46, 821-827.	3.0	42
16	Structural Properties of Carbon Nanogears. Fullerenes Nanotubes and Carbon Nanostructures, 2008, 16, 30-39.	2.1	1
17	Monte Carlo geometry optimization of Sin (n â©½ 71) clusters. Journal of Computational Methods in Sciences and Engineering, 2008, 7, 233-240.	0.2	0
18	Structural properties of lithium clusters: A Monte Carlo application. Journal of Computational Methods in Sciences and Engineering, 2008, 7, 409-416.	0.2	0

#	ARTICLE	IF	CITATIONS
19	IMPACT OF GEOMETRY ON THE HYDROGEN STORAGE PROPERTIES OF TITANIUM CARBIDE: A DFT STUDY ON THE MODEL TiC₄H₄. International Journal of Modern Physics C, 2007, 18, 1951-1960.	1.7	0
20	STRUCTURAL, ELECTRONIC AND QSAR PROPERTIES OF THE CYFLUTHRIN MOLECULE: A THEORETICAL AM1 AND PM3 TREATMENT. International Journal of Modern Physics C, 2006, 17, 1391-1402.	1.7	5
21	Comment on â€˜Modelling complexes of H2 molecules in fullerenesâ€™ by H. Dodziuk [Chem. Phys. Lett. 410 (2005) 39]. Chemical Physics Letters, 2006, 426, 222-223.	2.6	17
22	STRUCTURAL AND ELECTRONIC PROPERTIES OF c-BN(110) SURFACE AND SURFACE POINT DEFECTS. International Journal of Modern Physics C, 2006, 17, 795-803.	1.7	6
23	STRUCTURAL AND ELECTRONIC PROPERTIES OF THE DPPC MOLECULE. International Journal of Modern Physics C, 2006, 17, 967-974.	1.7	1
24	STRUCTURAL PROPERTIES OF COPPER NANOPARTICLES: MODIFIED DIFFUSION MONTE CARLO SIMULATIONS. International Journal of Modern Physics C, 2006, 17, 1171-1177.	1.7	2
25	STRUCTURAL AND ELECTRONIC PROPERTIES OF DIPROPYL SULFIDE: A THEORETICAL INVESTIGATION. International Journal of Modern Physics C, 2006, 17, 1179-1190.	1.7	1
26	SINGLE WALL BAMBOO SHAPED CARBON NANOTUBE: A MOLECULAR DYNAMICS AND ELECTRONIC STUDY. International Journal of Modern Physics C, 2006, 17, 187-196.	1.7	2
27	Structural and electronic properties of single-wall ZnO nanotubes. Physica E: Low-Dimensional Systems and Nanostructures, 2005, 28, 162-170.	2.7	56
28	Theoretical investigation of sulforaphane molecule. Computational and Theoretical Chemistry, 2005, 714, 81-85.	1.5	5
29	Cluster, Surface and Bulk Properties of ZnCd Binary Alloys: Molecular-Dynamics Simulations. Materials Science Forum, 2005, 502, 51-56.	0.3	1
30	JUNCTION FORMATION IN CROSSED NANOTUBES UNDER PRESSURE: MOLECULAR-DYNAMICS SIMULATIONS. International Journal of Modern Physics C, 2005, 16, 1371-1377.	1.7	4
31	METAL ATOM ENDOHEDRALLY DOPED C20 CAGE STRUCTURE: (X@C20; X =Ni, Fe, Co). International Journal of Modern Physics C, 2005, 16, 1553-1560.	1.7	2
32	THERMAL STABILITY OF BENZOROD ARRAYS: MOLECULAR-DYNAMICS SIMULATIONS. International Journal of Modern Physics C, 2005, 16, 827-834.	1.7	1
33	STRUCTURAL AND ELECTRONIC PROPERTIES OF (CnLi)+ CLUSTER IONS. International Journal of Modern Physics C, 2005, 16, 271-280.	1.7	1
34	AN ALGORITHM TO GENERATE TOROIDAL AND HELICAL CAGE STRUCTURES USING PENTAGONS, HEXAGONS AND HEPTAGONS. International Journal of Modern Physics C, 2004, 15, 267-278.	1.7	6
35	A COMPARATIVE STUDY OF EMPIRICAL POTENTIAL ENERGY FUNCTIONS: APPLICATIONS TO SILICON MICROCLUSTERS. International Journal of Modern Physics C, 2004, 15, 403-408.	1.7	2
36	Molecular-dynamics simulations of surface and bulk properties of Zn, Cd, and ZnCd systems. Physica Status Solidi (B): Basic Research, 2004, 241, 292-297.	1.5	6

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37	Theoretical investigation of quercetin and its radical isomers. Computational and Theoretical Chemistry, 2003, 631, 141-146.	1.5	47
38	AM1 treatment of endohedrally hydrogen doped fullerene, nH2@C60. Computational and Theoretical Chemistry, 2003, 638, 37-40.	1.5	52
39	Ammonia deposition in fullerene: (NH3)n@C60. Computational and Theoretical Chemistry, 2003, 640, 57-61.	1.5	28
40	STRUCTURAL FEATURES AND ENERGETICS OF ZnkCdl MICROCLUSTERS. International Journal of Modern Physics C, 2003, 14, 905-910.	1.7	9
41	AlTiNi Ternary Alloy Clusters:Â Molecular Dynamics Simulations and Density Functional Theory Calculations. Journal of Physical Chemistry B, 2003, 107, 12118-12125.	2.6	26
42	Application of Genetic Algorithms to Geometry Optimization of Microclusters: A Comparative Study of Empirical Potential Energy Functions for Silicon. Materials and Manufacturing Processes, 2003, 18, 329-339.	4.7	16
43	Structural features and energetics ofZnnâ^'mCdm(n=7,8)microclusters andZn50,Cd50,andZn25Cd25nanoparticles: Molecular-dynamics simulations. Physical Review A, 2003, 68, .	2.5	12
44	STRUCTURAL PROPERTIES OF DIAMOND NANORODS: MOLECULAR-DYNAMICS SIMULATIONS. International Journal of Modern Physics C, 2003, 14, 441-447.	1.7	9
45	STRUCTURAL AND ELECTRONIC PROPERTIES OF AlP DOPED HÃœCKEL TYPE CYCLACENE WITH FOUR BENZENOID RINGS. International Journal of Modern Physics C, 2003, 14, 1183-1189.	1.7	2
46	STRUCTURAL AND ELECTRONIC PROPERTIES OF MAGNESIUM DIBORIDE. International Journal of Modern Physics C, 2003, 14, 483-489.	1.7	4
47	Structural and electronic properties ofAlkTilNimmicroclusters: Density-functional-theory calculations. Physical Review A, 2002, 66, .	2.5	29
48	GOLD DEPOSITION ON GaAs(001) SURFACES: MOLECULAR-DYNAMICS SIMULATIONS. International Journal of Modern Physics C, 2002, 13, 759-769.	1.7	3
49	DECOMPOSITION OF SiH4 ON THE SA TYPE STEPPED Si(100) SURFACE. Surface Review and Letters, 2002, 09, 1401-1407.	1.1	4
50	STRUCTURAL PROPERTIES OF CARBON NANORODS: MOLECULAR-DYNAMICS SIMULATIONS. International Journal of Modern Physics C, 2002, 13, 367-373.	1.7	14
51	SIMULATION OF THE CASIMIRâ€"POLDER EFFECT FOR VARIOUS GEOMETRIES. International Journal of Modern Physics C, 2002, 13, 979-985.	1.7	2
52	Stability of Carbon Nanoonion C20@C60@C240:â€‰ Molecular Dynamics Simulations. Nano Letters, 2002, 2, 215-217.	9.1	13
53	Theoretical investigation of flavonoids naringenin and genistein. Computational and Theoretical Chemistry, 2002, 583, 163-167.	1.5	11
54	Structural and electronic properties of xanthohumol metabolite. Computational and Theoretical Chemistry, 2002, 583, 169-172.	1.5	5

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55	EMPIRICAL POTENTIAL ENERGY FUNCTIONS USED IN THE SIMULATIONS OF MATERIALS PROPERTIES. , 2001, , 1-103.		27
56	Energetics and stability of discrete charge distribution on a conducting disk. Physics Letters, Section A: General, Atomic and Solid State Physics, 2001, 290, 28-34.	2.1	8
57	STRUCTURAL AND ELECTRONIC PROPERTIES OF CARBON NANOBALLS: C20, C60, AND C20@C60. International Journal of Modern Physics C, 2001, 12, 1391-1399.	1.7	2
58	ADSORPTION OF WATER ON SINGLE AND DOUBLE LAYER STEPPED Si(100) SURFACES. Surface Review and Letters, 2001, 08, 251-259.	1.1	0
59	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
60	ADSORPTION OF HYDROGEN AND OXYGEN ON SINGLE AND DOUBLE LAYER STEPPED SI(100) SURFACES. International Journal of Modern Physics B, 2001, 15, 2261-2274.	2.0	1
61	ENERGETICS AND STABILITY OF DISCRETE CHARGE DISTRIBUTION ON THE SURFACE OF A SPHERE. International Journal of Modern Physics C, 2001, 12, 293-305.	1.7	4
62	MOLECULAR-DYNAMICS SIMULATIONS OF CARBON NANOCAGE STRUCTURES: NANOBALLS AND NANOTOROIDS. International Journal of Modern Physics C, 2001, 12, 685-690.	1.7	4
63	OPTICAL TRANSITIONS IN A PARABOLIC GaAs/Ga1-xAlxAs SUPERLATTICES. Surface Review and Letters, 2001, 08, 321-325.	1.1	0
64	ELECTRONIC BAND STRUCTURE OF STEPPED Si(100) SURFACES. Surface Review and Letters, 2001, 08, 61-66.	1.1	2
65	Zirconium microclusters: molecular-dynamics simulations and density functional calculations. Physica E: Low-Dimensional Systems and Nanostructures, 2000, 8, 223-229.	2.7	8
66	Stability of gold clusters: molecular-dynamics simulations. Physica E: Low-Dimensional Systems and Nanostructures, 2000, 8, 210-218.	2.7	44
67	GENERAL ANALYTIC DENSITY DISTRIBUTION FUNCTION FOR ATOMS. International Journal of Modern Physics C, 2000, 11, 1167-1177.	1.7	0
68	FROM CARBON NANOTUBES TO CARBON NANORODS. International Journal of Modern Physics C, 2000, 11, 1247-1255.	1.7	14
69	DECOMPOSITION OF C60 MOLECULES ON Si(100)(2 Ã— 1) SURFACE. International Journal of Modern Physics C, 2000, 11, 1067-1076.	1.7	1
70	MELTING AND FRAGMENTATION OF NICKEL NANOPARTICLES: MOLECULARâ€“DYNAMICS SIMULATIONS. International Journal of Modern Physics C, 2000, 11, 1567-1580.	1.7	9
71	STRUCTURAL AND ELECTRONIC PROPERTIES OF CARBON NANOTUBES. International Journal of Modern Physics C, 2000, 11, 175-182.	1.7	15
72	THE EFFECT OF PBC ON THE SIMULATION OF NANOTUBES. International Journal of Modern Physics C, 2000, 11, 547-551.	1.7	5

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73	MOLECULAR-DYNAMICS SIMULATIONS OF NICKEL CLUSTERS. International Journal of Modern Physics C, 2000, 11, 1013-1024.	1.7	6
74	MOLECULAR-DYNAMICS SIMULATION OF STEPPED Si(100) SURFACE. International Journal of Modern Physics C, 2000, 11, 999-1011.	1.7	1
75	MOLECULAR-DYNAMICS SIMULATION OF RADIATION DAMAGE ON COPPER CLUSTERS. International Journal of Modern Physics C, 2000, 11, 1025-1032.	1.7	1
76	ENERGETICS OF ARSENIC TERMINATED GaAs(001) SURFACES. International Journal of Modern Physics C, 2000, 11, 1225-1237.	1.7	4
77	Molecular-dynamics simulations of gold clusters. Advances in Quantum Chemistry, 2000, , 353-364.	0.8	4
78	Monte Carlo computer simulation of copper clusters. Physical Review A, 1999, 60, 3053-3057.	2.5	48
79	Molecular-dynamics simulations of silver clusters. Physica E: Low-Dimensional Systems and Nanostructures, 1999, 5, 1-6.	2.7	27
80	Energetics and structural stability of lanthanum microclusters. Chemical Physics Letters, 1999, 314, 203-209.	2.6	21
81	Molecular-Dynamics Simulations of Uranium Microclusters. Journal of the Physical Society of Japan, 1999, 68, 440-445.	1.6	9
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