OÄuz GÃ¼lseren

List of Publications by Year
in descending order

107	5,128	126708	88477
papers	citations	33 h-index	70 g-index

107	107	107	5407
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Theoretical study of germanium nanoclusters: significance of surface passivation. European Physical Journal Plus, 2022, 137, 1.	1.2	0
2	Tailoring Vibrational Signature and Functionality of 2D-Ordered Linear-Chain Carbon-Based Nanocarriers for Predictive Performance Enhancement of High-End Energetic Materials. Nanomaterials, 2022, 12, 1041.	1.9	2
3	Elucidating the Barriers on Direct Water Splitting: Key Role of Oxygen Vacancy Density and Coordination over PbTiO₃ and TiO₂. Journal of Physical Chemistry C, 2021, 125, 1874-1880.	1.5	5
4	A systematical ab-initio review of promising 2D MXene monolayers towards Li-ion battery applications. JPhys Energy, 2020, 2, 032006.	2.3	34
5	Temperature-dependent phonon spectrum of transition metal dichalcogenides calculated from the spectral energy density: Lattice thermal conductivity as an application. Physical Review B, 2019, 100, .	1.1	21
6	Double Perovskite Structure Induced by Co Addition to PbTiO₃: Insights from DFT and Experimental Solid-State NMR Spectroscopy. Journal of Physical Chemistry C, 2019, 123, 27132-27139.	1.5	8
7	Nanotribological Properties of the h-BN/Au(111) Interface: A DFT Study. Journal of Physical Chemistry C, 2019, 123, 28411-28418.	1.5	10
8	Local entanglement and string order parameter in dimerized models. Journal of Physics Condensed Matter, 2019, 31, 505602.	0.7	6
9	Deterministic phase transitions and self-organization in logistic cellular automata. Physical Review E, 2019, 100, 042216.	0.8	2
10	Alkali Metal Intercalation in MXene/Graphene Heterostructures: A New Platform for Ion Battery Applications. Journal of Physical Chemistry Letters, 2019, 10, 727-734.	2.1	88
11	Distributed contact flip chip InGaN/GaN blue LED; comparison with conventional LEDs. Superlattices and Microstructures, 2019, 128, 9-13.	1.4	12
12	Functionalization of (n, 0) CNTs (n = 3â€“16) by uracil: DFT studies. European Physical Journal B, 2018, 91, 1.	0.6	7
13	MXenes/graphene heterostructures for Li battery applications: a first principles study. Journal of Materials Chemistry A, 2018, 6, 2337-2345.	5.2	173
14	In pursuit of barrierless transition metal dichalcogenides lateral heterojunctions. Nanotechnology, 2018, 29, 295202.	1.3	6
15	First-principles investigation of armchair stanene nanoribbons. Physics Letters, Section A: General, Atomic and Solid State Physics, 2018, 382, 180-185.	0.9	19
16	A distinct correlation between the vibrational and thermal transport properties of group VA monolayer crystals. Nanoscale, 2018, 10, 7803-7812.	2.8	35
17	Validation of inter-atomic potential for WS2 and WSe2 crystals through assessment of thermal transport properties. Computational Materials Science, 2018, 144, 92-98.	1.4	36
18	Chemically uracilâ€“functionalized carbon and silicon carbide nanotubes: Computational studies. Materials Chemistry and Physics, 2018, 205, 164-170.	2.0	12

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19	Mixed ab initio and semiempirical study of hydrogen-terminated finite germanium nanowires. European Physical Journal Plus, 2018, 133, 1.	1.2	3
20	Scattering analysis of silver nanoparticles for solar cell applications using integral equations. , 2018, , .		0
21	Rich complex behaviour of self-assembled nanoparticles far from equilibrium. Nature Communications, 2017, 8, 14942.	5.8	40
22	DFT Studies of Graphene-Functionalised Derivatives of Capecitabine. Zeitschrift Fur Naturforschung - Section A Journal of Physical Sciences, 2017, 72, 1131-1138.	0.7	11
23	Gate induced monolayer behavior in twisted bilayer black phosphorus. 2D Materials, 2017, 4, 035025.	2.0	18
24	Structural and electronic properties of MoS2, WS2, and WS2/MoS2 heterostructures encapsulated with hexagonal boron nitride monolayers. Journal of Applied Physics, 2017, 122, .	1.1	49
25	Investigation of new two-dimensional materials derived from stanene. Computational Materials Science, 2017, 137, 208-214.	1.4	23
26	On the structural and electronic properties of Ir-silicide nanowires on Si(001) surface. Journal of Applied Physics, 2016, 120, .	1.1	8
27	Relaxations of fluorouracil tautomers by decorations of fullerene-like SiCs: DFT studies. Physics Letters, Section A: General, Atomic and Solid State Physics, 2016, 380, 2160-2166.	0.9	42
28	Systematic spatial and stoichiometric screening towards understanding the surface of ultrasmall oxygenated silicon nanocrystal. Applied Surface Science, 2016, 387, 771-778.	3.1	1
29	DFT explorations of quadrupole coupling constants for planar 5-fluorouracil pairs. Computational and Theoretical Chemistry, 2016, 1090, 67-73.	1.1	35
30	Peculiar Piezoelectric Properties of Soft Two-Dimensional Materials. Journal of Physical Chemistry C, 2016, 120, 13948-13953.	1.5	50
31	Mo₂C as a high capacity anode material: a first-principles study. Journal of Materials Chemistry A, 2016, 4, 6029-6035.	5.2	249
32	Anatase TiO2 nanowires functionalized by organic sensitizers for solar cells: A screened Coulomb hybrid density functional study. Journal of Applied Physics, 2015, 118, 194301.	1.1	5
33	DFT studies of CNTâ€“functionalized uracil-acetate hybrids. Physica E: Low-Dimensional Systems and Nanostructures, 2015, 73, 105-109.	1.3	8
34	Hybrid functional calculated optical and electronic structures of thin anatase TiO2 nanowires with organic dye adsorbates. Applied Surface Science, 2015, 354, 437-442.	3.1	3
35	Non-covalent functionalization of single wall carbon nanotubes and graphene by a conjugated polymer. Applied Physics Letters, 2014, 105, .	1.5	21
36	Range-Separated Hybrid Density Functional Study of Organic Dye Sensitizers on Anatase TiO₂ Nanowires. Journal of Physical Chemistry C, 2014, 118, 24776-24783.	1.5	2

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37	Electronic structures and optical spectra of thin anatase<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mi>TiO</mml:mi><mml:mn>2</mml:mn></mml:msub></m through hybrid density functional and quasiparticle calculations. Physical Review B, 2014, 89, .	1.1	14
38	Synthesis of Phosphorus Included Multiwalled Carbon Nanotubes by Pyrolysis of Sucrose. Journal of Physical Chemistry C, 2013, 117, 24554-24560.	1.5	3
39	An experimental and first-principles study of the effect of B/N doping in TiO2 thin films for visible light photo-catalysis. Journal of Photochemistry and Photobiology A: Chemistry, 2013, 254, 25-34.	2.0	27
40	Hall conductance in graphene with point defects. Journal of Physics Condensed Matter, 2013, 25, 055302.	0.7	2
41	Understanding the plasmonic properties of dewetting formed Ag nanoparticles for large area solar cell applications. Optics Express, 2013, 21, 18344.	1.7	47
42	The integer quantum Hall effect of a square lattice with an array of point defects. Journal of Physics Condensed Matter, 2012, 24, 345501.	0.7	3
43	Thermoelectric efficiency of nanowires with long-range surface disorder. Physical Review B, 2012, 85, .	1.1	4
44	Adsorption of Pt and Bimetallic PtAu Clusters on the Partially Reduced Rutile (110) TiO₂ Surface: A First-Principles Study. Journal of Physical Chemistry C, 2012, 116, 5735-5746.	1.5	40
45	Analysis of Charge Transfer for in Situ Li Intercalated Carbon Nanotubes. Journal of Physical Chemistry C, 2012, 116, 11364-11369.	1.5	25
46	DFT study of noble metal impurities on TiO2(110). European Physical Journal B, 2012, 85, 1.	0.6	12
47	Ab initiostudy of neutral (TiO₂)_nclusters and their interactions with water and transition metal atoms. Journal of Physics Condensed Matter, 2012, 24, 305301.	0.7	27
48	First-Principles Investigation of NO_x and SO_x Adsorption on Anatase-Supported BaO and Pt Overlayers. Journal of Physical Chemistry C, 2012, 116, 6191-6199.	1.5	20
49	Hofstadter butterfly of graphene with point defects. Physical Review B, 2012, 85, .	1.1	9
50	Interaction of BrPDI, BrGly, and BrAsp with the Rutile TiO2(110) Surface for Photovoltaic and Photocatalytic Applications: A First-Principles Study. Journal of Physical Chemistry C, 2011, 115, 9220-9226.	1.5	7
51	Effect of impurities on the mechanical and electronic properties of Au, Ag, and Cu monatomic chain nanowires. Physical Review B, 2011, 84, .	1.1	30
52	Bias in bonding behavior among boron, carbon, and nitrogen atoms in ion implanted a-BN, a-BC, and diamond like carbon films. Journal of Applied Physics, 2011, 110, .	1.1	20
53	An experimental and theoretical examination of the effect of sulfur on the pyrolytically grown carbon nanotubes from sucrose-based solid state precursors. Carbon, 2011, 49, 508-517.	5.4	20
54	Electronic structure of half-metallic ferromagnet Co2MnSi at high-pressure. European Physical Journal B, 2010, 76, 321-326.	0.6	19

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55	New Trends in Nanotribology. Tribology Letters, 2010, 39, 227-227.	1.2	1
56	DIPEPTIDE ADSORPTION ON Si(100)-2 Ã— 1 ASYMMETRIC SURFACE BY FIRST PRINCIPLES. International Journal of Modern Physics C, 2010, 21, 97-106.	0.8	1
57	Dye adsorbates BrPDI, BrGly, and BrAsp on anataseTiO2(001)for dye-sensitized solar cell applications. Physical Review B, 2009, 80, .	1.1	25
58	First-principles study of thin<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow><mml:mtext>TiO</mml:mtext></mml:mrow><mml:mi>x</mml:mi></mml:msub bulklike rutile nanowires. Physical Review B, 2009, 80, .	1.1	21
59	Modification of<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow><mml:mtext>TiO</mml:mtext></mml:mrow><mml:mn>2</mml:mn></mml:mst electronic structure by Au impurity investigated with density functional theory. Physical Review B, 2009, 80, .	1.1	16
60	VIBRATIONAL MODES IN SMALL Agn, Aun CLUSTERS: A FIRST PRINCIPLE CALCULATION. International Journal of Modern Physics B, 2009, 23, 5819-5834.	1.0	10
61	Characterization of platinum nitride from first-principles calculations. Journal of Physics Condensed Matter, 2009, 21, 485403.	0.7	10
62	Theoretical and spectroscopic investigations on the structure and bonding in Bâ€“Câ€“N thin films. Thin Solid Films, 2009, 518, 1459-1464.	0.8	18
63	First-principles investigation of pentagonal and hexagonal core-shell silicon nanowires with various core compositions. Physical Review B, 2009, 80, .	1.1	22
64	First principles study of structural phase stability of wide-gap semiconductors MgTe, MgS and MgSe. Computational Materials Science, 2009, 47, 593-598.	1.4	71
65	Pt-incorporated anatase<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow><mml:mtext>TiO</mml:mtext></mml:mrow><mml:mn>2</mml:mn></mml:mst for solar cell applications: First-principles density functional theory calculations. Physical Review B, 2009, 79, .	1.1	28
66	Infrared spectrum and STM images of cyclohexene-2-ethanamine: First principle investigation. Journal of Molecular Structure, 2008, 886, 144-147.	1.8	0
67	Analysis of defects on BN nano-structures using high-resolution electron microscopy and density-functional calculations. Ultramicroscopy, 2008, 108, 1484-1489.	0.8	4
68	Ab-initio Atomic Scale Study of Nearly Frictionless Surfaces. , 2007, , 57-77.		2
69	Effect of Molecular and Electronic Structure on the Light-Harvesting Properties of Dye Sensitizers. Journal of Physical Chemistry C, 2007, 111, 7539-7547.	1.5	22
70	Pattern information extraction from crystal structures. Computer Physics Communications, 2007, 176, 486-506.	3.0	1
71	First principles study of electronic and mechanical properties of molybdenum selenide type nanowires. Physical Review B, 2006, 74, .	1.1	26
72	First principles force field for metallic tantalum. Modelling and Simulation in Materials Science and Engineering, 2004, 12, S445-S459.	0.8	34

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73	Functionalized carbon nanotubes and device applications. Journal of Physics Condensed Matter, 2004, 16, R901-R960.	0.7	104
74	Energetics and Electronic Structures of Individual Atoms Adsorbed on Carbon Nanotubes. Journal of Physical Chemistry B, 2004, 108, 575-582.	1.2	116
75	Systematic study of adsorption of single atoms on a carbon nanotube. Physical Review B, 2003, 67, .	1.1	305
76	A comparative study of O2 adsorbed carbon nanotubes. Chemical Physics Letters, 2003, 380, 1-5.	1.2	30
77	Oxygenation of carbon nanotubes:â€ƒAtomic structure, energetics, and electronic structure. Physical Review B, 2003, 67, .	1.1	109
78	Electronic structure of the contact between carbon nanotube and metal electrodes. Applied Physics Letters, 2003, 83, 3180-3182.	1.5	61
79	Formation of quantum structures on a single nanotube by modulating hydrogen adsorption. Physical Review B, 2003, 68, .	1.1	29
80	Vacancy formation enthalpy at high pressures in tantalum. Journal of Physics Condensed Matter, 2003, 15, 855-861.	0.7	24
81	High-pressure thermoelasticity of body-centered-cubic tantalum. Physical Review B, 2002, 65, .	1.1	122
82	Reversible band-gap engineering in carbon nanotubes by radial deformation. Physical Review B, 2002, 65, .	1.1	121
83	First-principles zone-center theory of superconductivity in MgB 2. Applied Physics A: Materials Science and Processing, 2002, 74, s945-s947.	1.1	2
84	A simple theory of 40K superconductivity in MgB2: first-principles calculations of Tc, its dependence on boron mass and pressure. Journal of Physics and Chemistry of Solids, 2002, 63, 2201-2206.	1.9	14
85	Pentagonal nanowires:â€ƒA first-principles study of the atomic and electronic structure. Physical Review B, 2002, 65, .	1.1	75
86	Systematicab initiostudy of curvature effects in carbon nanotubes. Physical Review B, 2002, 65, .	1.1	235
87	Effects of hydrogen adsorption on single-wall carbon nanotubes: Metallic hydrogen decoration. Physical Review B, 2002, 66, .	1.1	104
88	Metal nanoring and tube formation on carbon nanotubes. Physical Review B, 2002, 66, .	1.1	33
89	PiezoelectricPb(Zr0.5Ti0.5)O3:â€ƒInterplay of atomic ordering, ferroelectric soft modes, and pressure. Physical Review B, 2002, 66, .	1.1	26
90	Giant Anharmonicity and Nonlinear Electron-Phonon Coupling inMgB2: A Combined First-Principles Calculation and Neutron Scattering Study. Physical Review Letters, 2001, 87, 037001.	2.9	381

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91	Tunable Adsorption on Carbon Nanotubes. Physical Review Letters, 2001, 87, 116802.	2.9	184
92	Exohydrogenated single-wall carbon nanotubes. Physical Review B, 2001, 64, .	1.1	103
93	Thermal equation of state of tantalum. Physical Review B, 2001, 63, .	1.1	87
94	Elasticity of iron at the temperature of the Earth's inner core. Nature, 2001, 413, 57-60.	13.7	240
95	Accuracy of equation-of-state formulations. American Mineralogist, 2000, 85, 338-344.	0.9	160
96	Variable and reversible quantum structures on a single carbon nanotube. Physical Review B, 2000, 62, R16345-R16348.	1.1	50
97	Pressure-induced interlinking of carbon nanotubes. Physical Review B, 2000, 62, 12648-12651.	1.1	116
98	Noncrystalline Structures of Ultrathin Unsupported Nanowires. Physical Review Letters, 1998, 80, 3775-3778.	2.9	269
99	Added row model ofTiO2(110)1Ã—2. Physical Review B, 1998, 58, 1586-1589.	1.1	132
100	Theoretical analysis of STM experiments at rutile TiO2 surfaces. Surface Science, 1997, 377-379, 150-154.	0.8	33
101	Premelting of thin wires. Physical Review B, 1995, 51, 7377-7380.	1.1	145
102	Localization of acoustical modes due to the electron-phonon interaction within a two-dimensional electron gas. Journal of Physics Condensed Matter, 1993, 5, 589-598.	0.7	9
103	Electric-field effects on finite-length superlattices. Physical Review B, 1992, 46, 7621-7626.	1.1	6
104	Electronic structure of a Si delta -layer embedded in Ge(001). Semiconductor Science and Technology, 1991, 6, 1002-1005.	1.0	1
105	Electronic structure of Ge-Si superlattices grown on Ge (001). Semiconductor Science and Technology, 1991, 6, 638-641.	1.0	1
106	Electronic structure of strained Sin/Gen(001) superlattices. Solid State Communications, 1988, 65, 1285-1290.	0.9	9
107	A study on the reconstruction of Ga terminated GaAs [1 1 1] surface. Solid State Communications, 1985, 56, 501-504.	0.9	7