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	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
2	Systematic study of adsorption of single atoms on a carbon nanotube. Physical Review B, 2003, 67, .	1.1	305
3	Noncrystalline Structures of Ultrathin Unsupported Nanowires. Physical Review Letters, 1998, 80, 3775-3778.	2.9	269
4	Mo₂C as a high capacity anode material: a first-principles study. Journal of Materials Chemistry A, 2016, 4, 6029-6035.	5.2	249
5	Elasticity of iron at the temperature of the Earth's inner core. Nature, 2001, 413, 57-60.	13.7	240
6	Systematicab initiostudy of curvature effects in carbon nanotubes. Physical Review B, 2002, 65, .	1.1	235
7	Tunable Adsorption on Carbon Nanotubes. Physical Review Letters, 2001, 87, 116802.	2.9	184
8	MXenes/graphene heterostructures for Li battery applications: a first principles study. Journal of Materials Chemistry A, 2018, 6, 2337-2345.	5.2	173
9	Accuracy of equation-of-state formulations. American Mineralogist, 2000, 85, 338-344.	0.9	160
10	Premelting of thin wires. Physical Review B, 1995, 51, 7377-7380.	1.1	145
11	Added row model ofTiO2(110)1Ã—2. Physical Review B, 1998, 58, 1586-1589.	1.1	132
12	High-pressure thermoelasticity of body-centered-cubic tantalum. Physical Review B, 2002, 65, .	1.1	122
13	Reversible band-gap engineering in carbon nanotubes by radial deformation. Physical Review B, 2002, 65, .	1.1	121
14	Pressure-induced interlinking of carbon nanotubes. Physical Review B, 2000, 62, 12648-12651.	1.1	116
15	Energetics and Electronic Structures of Individual Atoms Adsorbed on Carbon Nanotubes. Journal of Physical Chemistry B, 2004, 108, 575-582.	1.2	116
16	Oxygenation of carbon nanotubes:â€ƒAtomic structure, energetics, and electronic structure. Physical Review B, 2003, 67, .	1.1	109
17	Effects of hydrogen adsorption on single-wall carbon nanotubes: Metallic hydrogen decoration. Physical Review B, 2002, 66, .	1.1	104
18	Functionalized carbon nanotubes and device applications. Journal of Physics Condensed Matter, 2004, 16, R901-R960.	0.7	104

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19	Exohydrogenated single-wall carbon nanotubes. Physical Review B, 2001, 64, .	1.1	103
20	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
21	Thermal equation of state of tantalum. Physical Review B, 2001, 63, .	1.1	87
22	Pentagonal nanowires:â€ƒA first-principles study of the atomic and electronic structure. Physical Review B, 2002, 65, .	1.1	75
23	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
24	Electronic structure of the contact between carbon nanotube and metal electrodes. Applied Physics Letters, 2003, 83, 3180-3182.	1.5	61
25	Variable and reversible quantum structures on a single carbon nanotube. Physical Review B, 2000, 62, R16345-R16348.	1.1	50
26	Peculiar Piezoelectric Properties of Soft Two-Dimensional Materials. Journal of Physical Chemistry C, 2016, 120, 13948-13953.	1.5	50
27	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
28	Understanding the plasmonic properties of dewetting formed Ag nanoparticles for large area solar cell applications. Optics Express, 2013, 21, 18344.	1.7	47
29	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
30	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
31	Rich complex behaviour of self-assembled nanoparticles far from equilibrium. Nature Communications, 2017, 8, 14942.	5.8	40
32	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
33	DFT explorations of quadrupole coupling constants for planar 5-fluorouracil pairs. Computational and Theoretical Chemistry, 2016, 1090, 67-73.	1.1	35
34	A distinct correlation between the vibrational and thermal transport properties of group VA monolayer crystals. Nanoscale, 2018, 10, 7803-7812.	2.8	35
35	First principles force field for metallic tantalum. Modelling and Simulation in Materials Science and Engineering, 2004, 12, S445-S459.	0.8	34
36	A systematical ab-initio review of promising 2D MXene monolayers towards Li-ion battery applications. JPhys Energy, 2020, 2, 032006.	2.3	34

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37	Theoretical analysis of STM experiments at rutile TiO2 surfaces. Surface Science, 1997, 377-379, 150-154.	0.8	33
38	Metal nanoring and tube formation on carbon nanotubes. Physical Review B, 2002, 66, .	1.1	33
39	A comparative study of O2 adsorbed carbon nanotubes. Chemical Physics Letters, 2003, 380, 1-5.	1.2	30
40	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
41	Formation of quantum structures on a single nanotube by modulating hydrogen adsorption. Physical Review B, 2003, 68, .	1.1	29
42	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:msu for solar cell applications: First-principles density functional theory calculations. Physical Review B, 2009, 79, .	1.1	28
43	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
44	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
45	PiezoelectricPb(Zr0.5Ti0.5)O3:â€ƒInterplay of atomic ordering, ferroelectric soft modes, and pressure. Physical Review B, 2002, 66, .	1.1	26
46	First principles study of electronic and mechanical properties of molybdenum selenide type nanowires. Physical Review B, 2006, 74, .	1.1	26
47	Dye adsorbates BrPDI, BrGly, and BrAsp on anataseTiO2(001)for dye-sensitized solar cell applications. Physical Review B, 2009, 80, .	1.1	25
48	Analysis of Charge Transfer for in Situ Li Intercalated Carbon Nanotubes. Journal of Physical Chemistry C, 2012, 116, 11364-11369.	1.5	25
49	Vacancy formation enthalpy at high pressures in tantalum. Journal of Physics Condensed Matter, 2003, 15, 855-861.	0.7	24
50	Investigation of new two-dimensional materials derived from stanene. Computational Materials Science, 2017, 137, 208-214.	1.4	23
51	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
52	First-principles investigation of pentagonal and hexagonal core-shell silicon nanowires with various core compositions. Physical Review B, 2009, 80, .	1.1	22
53	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:mn>2</mml:mn></mml:msub> bulklike rutile nanowires. Physical Review B, 2009, 80, .	1.1	21
54	Non-covalent functionalization of single wall carbon nanotubes and graphene by a conjugated polymer. Applied Physics Letters, 2014, 105, .	1.5	21

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55	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
56	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
57	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
58	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
59	Electronic structure of half-metallic ferromagnet Co2MnSi at high-pressure. European Physical Journal B, 2010, 76, 321-326.	0.6	19
60	First-principles investigation of armchair stanene nanoribbons. Physics Letters, Section A: General, Atomic and Solid State Physics, 2018, 382, 180-185.	0.9	19
61	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
62	Gate induced monolayer behavior in twisted bilayer black phosphorus. 2D Materials, 2017, 4, 035025.	2.0	18
63	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:msub></mml:mrow></mml:math> electronic structure by Au impurity investigated with density functional theory. Physical Review B, 2009, 80, .	1.1	16
64	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
65	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></mml:math> through hybrid density functional and quasiparticle calculations. Physical Review B, 2014, 89, .	1.1	14
66	DFT study of noble metal impurities on TiO2(110). European Physical Journal B, 2012, 85, 1.	0.6	12
67	Chemically uracilâ€“functionalized carbon and silicon carbide nanotubes: Computational studies. Materials Chemistry and Physics, 2018, 205, 164-170.	2.0	12
68	Distributed contact flip chip InGaN/GaN blue LED; comparison with conventional LEDs. Superlattices and Microstructures, 2019, 128, 9-13.	1.4	12
69	DFT Studies of Graphene-Functionalised Derivatives of Capecitabine. Zeitschrift Fur Naturforschung - Section A Journal of Physical Sciences, 2017, 72, 1131-1138.	0.7	11
70	VIBRATIONAL MODES IN SMALL Agn, Aun CLUSTERS: A FIRST PRINCIPLE CALCULATION. International Journal of Modern Physics B, 2009, 23, 5819-5834.	1.0	10
71	Characterization of platinum nitride from first-principles calculations. Journal of Physics Condensed Matter, 2009, 21, 485403.	0.7	10
72	Nanotribological Properties of the h-BN/Au(111) Interface: A DFT Study. Journal of Physical Chemistry C, 2019, 123, 28411-28418.	1.5	10

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73	Electronic structure of strained Sin/Gen(001) superlattices. Solid State Communications, 1988, 65, 1285-1290.	0.9	9
74	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
75	Hofstadter butterfly of graphene with point defects. Physical Review B, 2012, 85, .	1.1	9
76	DFT studies of CNTâ€“functionalized uracil-acetate hybrids. Physica E: Low-Dimensional Systems and Nanostructures, 2015, 73, 105-109.	1.3	8
77	On the structural and electronic properties of Ir-silicide nanowires on Si(001) surface. Journal of Applied Physics, 2016, 120, .	1.1	8
78	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
79	A study on the reconstruction of Ga terminated GaAs [1 1 1] surface. Solid State Communications, 1985, 56, 501-504.	0.9	7
80	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
81	Functionalization of (n, 0) CNTs (n = 3â€“16) by uracil: DFT studies. European Physical Journal B, 2018, 91, 1.	0.6	7
82	Electric-field effects on finite-length superlattices. Physical Review B, 1992, 46, 7621-7626.	1.1	6
83	In pursuit of barrierless transition metal dichalcogenides lateral heterojunctions. Nanotechnology, 2018, 29, 295202.	1.3	6
84	Local entanglement and string order parameter in dimerized models. Journal of Physics Condensed Matter, 2019, 31, 505602.	0.7	6
85	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
86	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
87	Analysis of defects on BN nano-structures using high-resolution electron microscopy and density-functional calculations. Ultramicroscopy, 2008, 108, 1484-1489.	0.8	4
88	Thermoelectric efficiency of nanowires with long-range surface disorder. Physical Review B, 2012, 85, .	1.1	4
89	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
90	Synthesis of Phosphorus Included Multiwalled Carbon Nanotubes by Pyrolysis of Sucrose. Journal of Physical Chemistry C, 2013, 117, 24554-24560.	1.5	3

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91	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
92	Mixed ab initio and semiempirical study of hydrogen-terminated finite germanium nanowires. European Physical Journal Plus, 2018, 133, 1.	1.2	3
93	First-principles zone-center theory of superconductivity in MgB 2. Applied Physics A: Materials Science and Processing, 2002, 74, s945-s947.	1.1	2
94	Ab-initio Atomic Scale Study of Nearly Frictionless Surfaces. , 2007, , 57-77.		2
95	Hall conductance in graphene with point defects. Journal of Physics Condensed Matter, 2013, 25, 055302.	0.7	2
96	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
97	Deterministic phase transitions and self-organization in logistic cellular automata. Physical Review E, 2019, 100, 042216.	0.8	2
98	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
99	Electronic structure of a Si delta -layer embedded in Ge(001). Semiconductor Science and Technology, 1991, 6, 1002-1005.	1.0	1
100	Electronic structure of Ge-Si superlattices grown on Ge (001). Semiconductor Science and Technology, 1991, 6, 638-641.	1.0	1
101	Pattern information extraction from crystal structures. Computer Physics Communications, 2007, 176, 486-506.	3.0	1
102	New Trends in Nanotribology. Tribology Letters, 2010, 39, 227-227.	1.2	1
103	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
104	Systematic spatial and stoichiometric screening towards understanding the surface of ultrasmall oxygenated silicon nanocrystal. Applied Surface Science, 2016, 387, 771-778.	3.1	1
105	Infrared spectrum and STM images of cyclohexene-2-ethanamine: First principle investigation. Journal of Molecular Structure, 2008, 886, 144-147.	1.8	0
106	Scattering analysis of silver nanoparticles for solar cell applications using integral equations. , 2018, , .		0
107	Theoretical study of germanium nanoclusters: significance of surface passivation. European Physical Journal Plus, 2022, 137, 1.	1.2	0