

# OÄuz GÃ¼lseren

## List of Publications by Year in descending order

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107  
papers

5,128  
citations

126858

33  
h-index

88593

70  
g-index

107  
all docs

107  
docs citations

107  
times ranked

5407  
citing authors

#	ARTICLE	IF	CITATIONS
1	Theoretical study of germanium nanoclusters: significance of surface passivation. <i>European Physical Journal Plus</i> , 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. <i>Nanomaterials</i> , 2022, 12, 1041.	1.9	2
3	Elucidating the Barriers on Direct Water Splitting: Key Role of Oxygen Vacancy Density and Coordination over $\text{PbTiO}_3$ and $\text{TiO}_2$ . <i>Journal of Physical Chemistry C</i> , 2021, 125, 1874-1880.	1.5	5
4	A systematical ab-initio review of promising 2D MXene monolayers towards Li-ion battery applications. <i>JPhys Energy</i> , 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. <i>Physical Review B</i> , 2019, 100, .	1.1	21
6	Double Perovskite Structure Induced by Co Addition to $\text{PbTiO}_3$ : Insights from DFT and Experimental Solid-State NMR Spectroscopy. <i>Journal of Physical Chemistry C</i> , 2019, 123, 27132-27139.	1.5	8
7	Nanotribological Properties of the h-BN/Au(111) Interface: A DFT Study. <i>Journal of Physical Chemistry C</i> , 2019, 123, 28411-28418.	1.5	10
8	Local entanglement and string order parameter in dimerized models. <i>Journal of Physics Condensed Matter</i> , 2019, 31, 505602.	0.7	6
9	Deterministic phase transitions and self-organization in logistic cellular automata. <i>Physical Review E</i> , 2019, 100, 042216.	0.8	2
10	Alkali Metal Intercalation in MXene/Graphene Heterostructures: A New Platform for Ion Battery Applications. <i>Journal of Physical Chemistry Letters</i> , 2019, 10, 727-734.	2.1	88
11	Distributed contact flip chip InGaN/GaN blue LED; comparison with conventional LEDs. <i>Superlattices and Microstructures</i> , 2019, 128, 9-13.	1.4	12
12	Functionalization of (n, 0) CNTs ( $n = 3 \leq 16$ ) by uracil: DFT studies. <i>European Physical Journal B</i> , 2018, 91, 1.	0.6	7
13	MXenes/graphene heterostructures for Li battery applications: a first principles study. <i>Journal of Materials Chemistry A</i> , 2018, 6, 2337-2345.	5.2	173
14	In pursuit of barrierless transition metal dichalcogenides lateral heterojunctions. <i>Nanotechnology</i> , 2018, 29, 295202.	1.3	6
15	First-principles investigation of armchair stanene nanoribbons. <i>Physics Letters, Section A: General, Atomic and Solid State Physics</i> , 2018, 382, 180-185.	0.9	19
16	A distinct correlation between the vibrational and thermal transport properties of group VA monolayer crystals. <i>Nanoscale</i> , 2018, 10, 7803-7812.	2.8	35
17	Validation of inter-atomic potential for $\text{WS}_2$ and $\text{WSe}_2$ crystals through assessment of thermal transport properties. <i>Computational Materials Science</i> , 2018, 144, 92-98.	1.4	36
18	Chemically uracil-functionalized carbon and silicon carbide nanotubes: Computational studies. <i>Materials Chemistry and Physics</i> , 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 MoS <sub>2</sub> , WS <sub>2</sub> , and WS <sub>2</sub> /MoS <sub>2</sub> 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	Mo <sub>2</sub> C as a high capacity anode material: a first-principles study. Journal of Materials Chemistry A, 2016, 4, 6029-6035.	5.2	249
32	Anatase TiO <sub>2</sub> 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 TiO <sub>2</sub> 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 TiO <sub>2</sub> 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 $\text{TiO}_2$ through hybrid density functional and quasiparticle calculations. <i>Physical Review B</i> , 2014, 89, .	1.5	14
38	Synthesis of Phosphorus Included Multiwalled Carbon Nanotubes by Pyrolysis of Sucrose. <i>Journal of Physical Chemistry C</i> , 2013, 117, 24554-24560.	1.5	3
39	An experimental and first-principles study of the effect of B/N doping in $\text{TiO}_2$ thin films for visible light photo-catalysis. <i>Journal of Photochemistry and Photobiology A: Chemistry</i> , 2013, 254, 25-34.	2.0	27
40	Hall conductance in graphene with point defects. <i>Journal of Physics Condensed Matter</i> , 2013, 25, 055302.	0.7	2
41	Understanding the plasmonic properties of dewetting formed Ag nanoparticles for large area solar cell applications. <i>Optics Express</i> , 2013, 21, 18344.	1.7	47
42	The integer quantum Hall effect of a square lattice with an array of point defects. <i>Journal of Physics Condensed Matter</i> , 2012, 24, 345501.	0.7	3
43	Thermoelectric efficiency of nanowires with long-range surface disorder. <i>Physical Review B</i> , 2012, 85, .	1.1	4
44	Adsorption of Pt and Bimetallic PtAu Clusters on the Partially Reduced Rutile (110) $\text{TiO}_2$ Surface: A First-Principles Study. <i>Journal of Physical Chemistry C</i> , 2012, 116, 5735-5746.	1.5	40
45	Analysis of Charge Transfer for in Situ Li Intercalated Carbon Nanotubes. <i>Journal of Physical Chemistry C</i> , 2012, 116, 11364-11369.	1.5	25
46	DFT study of noble metal impurities on $\text{TiO}_2(110)$ . <i>European Physical Journal B</i> , 2012, 85, 1.	0.6	12
47	Ab initio study of neutral ( $\text{TiO}_2$ ) <sub>n</sub> clusters and their interactions with water and transition metal atoms. <i>Journal of Physics Condensed Matter</i> , 2012, 24, 305301.	0.7	27
48	First-Principles Investigation of $\text{NO}_x$ and $\text{SO}_x$ Adsorption on Anatase-Supported BaO and Pt Overlayers. <i>Journal of Physical Chemistry C</i> , 2012, 116, 6191-6199.	1.5	20
49	Hofstadter butterfly of graphene with point defects. <i>Physical Review B</i> , 2012, 85, .	1.1	9
50	Interaction of BrPDI, BrGly, and BrAsp with the Rutile $\text{TiO}_2(110)$ Surface for Photovoltaic and Photocatalytic Applications: A First-Principles Study. <i>Journal of Physical Chemistry C</i> , 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. <i>Physical Review B</i> , 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. <i>Journal of Applied Physics</i> , 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. <i>Carbon</i> , 2011, 49, 508-517.	5.4	20
54	Electronic structure of half-metallic ferromagnet $\text{Co}_2\text{MnSi}$ at high-pressure. <i>European Physical Journal B</i> , 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 $\text{Si}(100)-2 \times 1$ 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 anatase $\text{TiO}_2(001)$ for dye-sensitized solar cell applications. Physical Review B, 2009, 80, .	1.1	25
58	First-principles study of thin $\text{TiO}_2$ bulklike rutile nanowires. Physical Review B, 2009, 80, .	1.1	16
59	Modification of $\text{TiO}_2$ electronic structure by Au impurity investigated with density functional theory. Physical Review B, 2009, 80, .	1.1	16
60	VIBRATIONAL MODES IN SMALL Ag <sub>n</sub> , Au <sub>n</sub> 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 $\text{Ba}_x\text{N}$ 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 $\text{TiO}_2$ 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 O <sub>2</sub> adsorbed carbon nanotubes. Chemical Physics Letters, 2003, 380, 1-5.	1.2	30
77	Oxygenation of carbon nanotubes: Atomic 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 <sub>2</sub> . Applied Physics A: Materials Science and Processing, 2002, 74, s945-s947.	1.1	2
84	A simple theory of 40K superconductivity in MgB <sub>2</sub> : first-principles calculations of T <sub>c</sub> , its dependence on boron mass and pressure. Journal of Physics and Chemistry of Solids, 2002, 63, 2201-2206.	1.9	14
85	Pentagonal nanowires: A 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)O <sub>3</sub> : Interplay of atomic ordering, ferroelectric soft modes, and pressure. Physical Review B, 2002, 66, .	1.1	26
90	Giant Anharmonicity and Nonlinear Electron-Phonon Coupling inMgB <sub>2</sub> : 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 of TiO <sub>2</sub> (110)1Å—2. Physical Review B, 1998, 58, 1586-1589.	1.1	132
100	Theoretical analysis of STM experiments at rutile TiO <sub>2</sub> 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 Si <sub>n</sub> /Ge <sub>n</sub> (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