Oguz Glseren

List of Publications by Citations

105 papers	4,393 citations	31 h-index	65 g-index
107 ext. papers	4,740 ext. citations	4 avg, IF	5.47 L-index

#	Paper	IF	Citations
105	Giant anharmonicity and nonlinear electron-phonon coupling in MgB2: a combined first-principles calculation and neutron scattering study. *Physical Review Letters*, **2001**, 87, 037001	7.4	328
104	Systematic study of adsorption of single atoms on a carbon nanotube. *Physical Review B*, **2003**, 67,	3.3	284
103	Noncrystalline Structures of Ultrathin Unsupported Nanowires. *Physical Review Letters*, **1998**, 80, 3775-3778	7.4	253
102	Elasticity of iron at the temperature of the Earth's inner core. *Nature*, **2001**, 413, 57-60	50.4	220
101	Systematic ab initio study of curvature effects in carbon nanotubes. *Physical Review B*, **2002**, 65,	3.3	202
100	Mo2C as a high capacity anode material: a first-principles study. *Journal of Materials Chemistry A*, **2016**, 4, 6029-6035	13	179
99	Tunable adsorption on carbon nanotubes. *Physical Review Letters*, **2001**, 87, 116802	7.4	169
98	Accuracy of equation-of-state formulations. *American Mineralogist*, **2000**, 85, 338-344	2.9	135
97	Premelting of thin wires. *Physical Review B*, **1995**, 51, 7377-7380	3.3	131
96	Added row model of TiO2(110)1□. *Physical Review B*, **1998**, 58, 1586-1589	3.3	121
95	MXenes/graphene heterostructures for Li battery applications: a first principles study. *Journal of Materials Chemistry A*, **2018**, 6, 2337-2345	13	119
94	Reversible band-gap engineering in carbon nanotubes by radial deformation. *Physical Review B*, **2002**, 65,	3.3	116
93	High-pressure thermoelasticity of body-centered-cubic tantalum. *Physical Review B*, **2002**, 65,	3.3	109
92	Energetics and Electronic Structures of Individual Atoms Adsorbed on Carbon Nanotubes. *Journal of Physical Chemistry B*, **2004**, 108, 575-582	3.4	108
91	Oxygenation of carbon nanotubes: Atomic structure, energetics, and electronic structure. *Physical Review B*, **2003**, 67,	3.3	106
90	Pressure-induced interlinking of carbon nanotubes. *Physical Review B*, **2000**, 62, 12648-12651	3.3	104
89	Effects of hydrogen adsorption on single-wall carbon nanotubes: Metallic hydrogen decoration. *Physical Review B*, **2002**, 66,	3.3	99

88	Exohydrogenated single-wall carbon nanotubes. *Physical Review B*, **2001**, 64,	3.3	94
87	Functionalized carbon nanotubes and device applications. *Journal of Physics Condensed Matter*, **2004**, 16, R901-R960	1.8	90
86	Thermal equation of state of tantalum. *Physical Review B*, **2001**, 63,	3.3	76
85	Pentagonal nanowires: A first-principles study of the atomic and electronic structure. *Physical Review B*, **2002**, 65,	3.3	72
84	First principles study of structural phase stability of wide-gap semiconductors MgTe, MgS and MgSe. *Computational Materials Science*, **2009**, 47, 593-598	3.2	63
83	Alkali Metal Intercalation in MXene/Graphene Heterostructures: A New Platform for Ion Battery Applications. *Journal of Physical Chemistry Letters*, **2019**, 10, 727-734	6.4	60
82	Electronic structure of the contact between carbon nanotube and metal electrodes. *Applied Physics Letters*, **2003**, 83, 3180-3182	3.4	52
81	Variable and reversible quantum structures on a single carbon nanotube. *Physical Review B*, **2000**, 62, R16345-R16348	3.3	49
80	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	3.8	36
79	First principles force field for metallic tantalum. *Modelling and Simulation in Materials Science and Engineering*, **2004**, 12, S445-S459	2	34
78	Understanding the plasmonic properties of dewetting formed Ag nanoparticles for large area solar cell applications. *Optics Express*, **2013**, 21, 18344-53	3.3	33
77	Theoretical analysis of STM experiments at rutile TiO2 surfaces. *Surface Science*, **1997**, 377-379, 150-154	1.8	33
76	Peculiar Piezoelectric Properties of Soft Two-Dimensional Materials. *Journal of Physical Chemistry C* , **2016**, 120, 13948-13953	3.8	32
75	Metal nanoring and tube formation on carbon nanotubes. *Physical Review B*, **2002**, 66,	3.3	31
74	Rich complex behaviour of self-assembled nanoparticles far from equilibrium. *Nature Communications*, **2017**, 8, 14942	17.4	29
73	Structural and electronic properties of MoS2, WS2, and WS2/MoS2 heterostructures encapsulated with hexagonal boron nitride monolayers. *Journal of Applied Physics*, **2017**, 122, 065303	2.5	29
72	Formation of quantum structures on a single nanotube by modulating hydrogen adsorption. *Physical Review B*, **2003**, 68,	3.3	29
71	Effect of impurities on the mechanical and electronic properties of Au, Ag, and Cu monatomic chain nanowires. *Physical Review B*, **2011**, 84,	3.3	28

70	A comparative study of O2 adsorbed carbon nanotubes. *Chemical Physics Letters*, **2003**, 380, 1-5	2.5	28
69	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	2.3	28
68	DFT explorations of quadrupole coupling constants for planar 5-fluorouracil pairs. *Computational and Theoretical Chemistry*, **2016**, 1090, 67-73	2	27
67	Pt-incorporated anatase TiO2(001) surface for solar cell applications: First-principles density functional theory calculations. *Physical Review B*, **2009**, 79,	3.3	27
66	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	4.7	25
65	Dye adsorbates BrPDI, BrGly, and BrAsp on anatase TiO2(001) for dye-sensitized solar cell applications. *Physical Review B*, **2009**, 80,	3.3	25
64	A distinct correlation between the vibrational and thermal transport properties of group VA monolayer crystals. *Nanoscale*, **2018**, 10, 7803-7812	7.7	23
63	Analysis of Charge Transfer for in Situ Li Intercalated Carbon Nanotubes. *Journal of Physical Chemistry C*, **2012**, 116, 11364-11369	3.8	23
62	Validation of inter-atomic potential for WS2 and WSe2 crystals through assessment of thermal transport properties. *Computational Materials Science*, **2018**, 144, 92-98	3.2	23
61	Ab initio study of neutral (TiO2)n clusters and their interactions with water and transition metal atoms. *Journal of Physics Condensed Matter*, **2012**, 24, 305301	1.8	22
60	Effect of Molecular and Electronic Structure on the Light-Harvesting Properties of Dye Sensitizers. *Journal of Physical Chemistry C*, **2007**, 111, 7539-7547	3.8	22
59	Piezoelectric Pb(Zr0.5Ti0.5)O3: Interplay of atomic ordering, ferroelectric soft modes, and pressure. *Physical Review B*, **2002**, 66,	3.3	22
58	First-principles study of thin TiOx and bulklike rutile nanowires. *Physical Review B*, **2009**, 80,	3.3	21
57	First principles study of electronic and mechanical properties of molybdenum selenide type nanowires. *Physical Review B*, **2006**, 74,	3.3	21
56	First-principles investigation of pentagonal and hexagonal core-shell silicon nanowires with various core compositions. *Physical Review B*, **2009**, 80,	3.3	20
55	Vacancy formation enthalpy at high pressures in tantalum. *Journal of Physics Condensed Matter*, **2003**, 15, 855-861	1.8	19
54	First-Principles Investigation of NOx and SOx Adsorption on Anatase-Supported BaO and Pt Overlayers. *Journal of Physical Chemistry C*, **2012**, 116, 6191-6199	3.8	18
53	Electronic structure of half-metallic ferromagnet Co2MnSi at high-pressure. *European Physical Journal B*, **2010**, 76, 321-326	1.2	18

52	Non-covalent functionalization of single wall carbon nanotubes and graphene by a conjugated polymer. *Applied Physics Letters*, **2014**, 105, 013103	3.4	17
51	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, 074906	2.5	17
50	Modification of TiO2(001) surface electronic structure by Au impurity investigated with density functional theory. *Physical Review B*, **2009**, 80,	3.3	15
49	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	10.4	15
48	First-principles investigation of armchair stanene nanoribbons. *Physics Letters, Section A: General, Atomic and Solid State Physics*, **2018**, 382, 180-185	2.3	14
47	Theoretical and spectroscopic investigations on the structure and bonding in B□□N thin films. *Thin Solid Films*, **2009**, 518, 1459-1464	2.2	14
46	Investigation of new two-dimensional materials derived from stanene. *Computational Materials Science*, **2017**, 137, 208-214	3.2	14
45	A systematical ab-initio review of promising 2D MXene monolayers towards Li-ion battery applications. *JPhys Energy*, **2020**, 2, 032006	4.9	14
44	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	3.9	13
43	Gate induced monolayer behavior in twisted bilayer black phosphorus. *2D Materials*, **2017**, 4, 035025	5.9	12
42	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,	3.3	11
41	Electronic structures and optical spectra of thin anatase TiO2 nanowires through hybrid density functional and quasiparticle calculations. *Physical Review B*, **2014**, 89,	3.3	11
40	DFT study of noble metal impurities on TiO2(110). *European Physical Journal B*, **2012**, 85, 1	1.2	11
39	DFT Studies of Graphene-Functionalised Derivatives of Capecitabine. *Zeitschrift Fur Naturforschung - Section A Journal of Physical Sciences*, **2017**, 72, 1131-1138	1.4	10
38	VIBRATIONAL MODES IN SMALL Agn, Aun CLUSTERS: A FIRST PRINCIPLE CALCULATION. *International Journal of Modern Physics B*, **2009**, 23, 5819-5834	1.1	10
37	Characterization of platinum nitride from first-principles calculations. *Journal of Physics Condensed Matter*, **2009**, 21, 485403	1.8	9
36	Electronic structure of strained Sin/Gen(001) superlattices. *Solid State Communications*, **1988**, 65, 1285-1290	2.0	9
35	Chemically uracil□unctionalized carbon and silicon carbide nanotubes: Computational studies. *Materials Chemistry and Physics*, **2018**, 205, 164-170	4.4	9

34	Hofstadter butterfly of graphene with point defects. *Physical Review B*, **2012**, 85,	3.3	8
33	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	1.8	8
32	On the structural and electronic properties of Ir-silicide nanowires on Si(001) surface. *Journal of Applied Physics*, **2016**, 120, 095303	2.5	8
31	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	3.8	7
30	A study on the reconstruction of Ga terminated GaAs [1 1 1] surface. *Solid State Communications*, **1985**, 56, 501-504	1.6	6
29	DFT studies of CNT-functionalized uracil-acetate hybrids. *Physica E: Low-Dimensional Systems and Nanostructures*, **2015**, 73, 105-109	3	5
28	Electric-field effects on finite-length superlattices. *Physical Review B*, **1992**, 46, 7621-7626	3.3	5
27	Anatase TiO2 nanowires functionalized by organic sensitizers for solar cells: A screened Coulomb hybrid density functional study. *Journal of Applied Physics*, **2015**, 118, 194301	2.5	4
26	Analysis of defects on BN nano-structures using high-resolution electron microscopy and density-functional calculations. *Ultramicroscopy*, **2008**, 108, 1484-9	3.1	4
25	Distributed contact flip chip InGaN/GaN blue LED; comparison with conventional LEDs. *Superlattices and Microstructures*, **2019**, 128, 9-13	2.8	4
24	Hybrid functional calculated optical and electronic structures of thin anatase TiO2 nanowires with organic dye adsorbates. *Applied Surface Science*, **2015**, 354, 437-442	6.7	3
23	In pursuit of barrierless transition metal dichalcogenides lateral heterojunctions. *Nanotechnology*, **2018**, 29, 295202	3.4	3
22	Nanotribological Properties of the h-BN/Au(111) Interface: A DFT Study. *Journal of Physical Chemistry C*, **2019**, 123, 28411-28418	3.8	3
21	Synthesis of Phosphorus Included Multiwalled Carbon Nanotubes by Pyrolysis of Sucrose. *Journal of Physical Chemistry C*, **2013**, 117, 24554-24560	3.8	3
20	The integer quantum Hall effect of a square lattice with an array of point defects. *Journal of Physics Condensed Matter*, **2012**, 24, 345501	1.8	3
19	Thermoelectric efficiency of nanowires with long-range surface disorder. *Physical Review B*, **2012**, 85,	3.3	3
18	Mixed ab initio and semiempirical study of hydrogen-terminated finite germanium nanowires. *European Physical Journal Plus*, **2018**, 133, 1	3.1	3
17	Functionalization of (n, 0) CNTs (n = 3–16) by uracil: DFT studies. *European Physical Journal B*, **2018**, 91, 1	1.2	2

List of Publications

16	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	3.8	2
15	Local entanglement and string order parameter in dimerized models. *Journal of Physics Condensed Matter*, **2019**, 31, 505602	1.8	2
14	Range-Separated Hybrid Density Functional Study of Organic Dye Sensitizers on Anatase TiO2 Nanowires. *Journal of Physical Chemistry C*, **2014**, 118, 24776-24783	3.8	2
13	Hall conductance in graphene with point defects. *Journal of Physics Condensed Matter*, **2013**, 25, 055302	1.8	2
12	Ab-initio Atomic Scale Study of Nearly Frictionless Surfaces **2007**, 57-77		2
11	First-principles zone-center theory of superconductivity in MgB2. *Applied Physics A: Materials Science and Processing*, **2002**, 74, s945-s947	2.6	2
10	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	3.8	2
9	Deterministic phase transitions and self-organization in logistic cellular automata. *Physical Review E* , **2019**, 100, 042216	2.4	1
8	Systematic spatial and stoichiometric screening towards understanding the surface of ultrasmall oxygenated silicon nanocrystal. *Applied Surface Science*, **2016**, 387, 771-778	6.7	1
7	DIPEPTIDE ADSORPTION ON Si(100)-2 □ ASYMMETRIC SURFACE BY FIRST PRINCIPLES. *International Journal of Modern Physics C*, **2010**, 21, 97-106	1.1	1
6	New Trends in Nanotribology. *Tribology Letters*, **2010**, 39, 227-227	2.8	1
5	Pattern information extraction from crystal structures. *Computer Physics Communications*, **2007**, 176, 486-506	4.2	1
4	Electronic structure of a Si delta -layer embedded in Ge(001). *Semiconductor Science and Technology* , **1991**, 6, 1002-1005	1.8	1
3	Electronic structure of Ge-Si superlattices grown on Ge (001). *Semiconductor Science and Technology*, **1991**, 6, 638-641	1.8	1
2	Infrared spectrum and STM images of cyclohexene-2-ethanamine: First principle investigation. *Journal of Molecular Structure*, **2008**, 886, 144-147	3.4	
1	Theoretical study of germanium nanoclusters: significance of surface passivation. *European Physical Journal Plus*, **2022**, 137, 1	3.1	