

Deniz Cakir

List of Publications by Year in descending order

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60
papers

2,983
citations

201385

27
h-index

161609

54
g-index

60
all docs

60
docs citations

60
times ranked

4357
citing authors

#	ARTICLE	IF	CITATIONS
1	Tuning of the electronic and optical properties of single-layer black phosphorus by strain. <i>Physical Review B</i> , 2014, 90, .	1.1	279
2	Mo ₂ C as a high capacity anode material: a first-principles study. <i>Journal of Materials Chemistry A</i> , 2016, 4, 6029-6035.	5.2	249
3	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
4	Promising Piezoelectric Performance of Single Layer Transition-Metal Dichalcogenides and Dioxides. <i>Journal of Physical Chemistry C</i> , 2015, 119, 23231-23237.	1.5	164
5	Mechanical and thermal properties of <i>h</i> -MX ₂ (M=Cr, Mo, W; X=O, S, Se, Te) monolayers: A comparative study. <i>Applied Physics Letters</i> , 2014, 104, 203110.	1.5	157
6	Significant effect of stacking on the electronic and optical properties of few-layer black phosphorus. <i>Physical Review B</i> , 2015, 92, .	1.1	152
7	Formation and stability of point defects in monolayer rhenium disulfide. <i>Physical Review B</i> , 2014, 89, .	1.1	151
8	Thermal properties of black and blue phosphorenes from a first-principles quasi-harmonic approach. <i>Physical Review B</i> , 2015, 92, .	1.1	140
9	The influence of surface functionalization on thermal transport and thermoelectric properties of MXene monolayers. <i>Nanoscale</i> , 2018, 10, 8859-8868.	2.8	118
10	Realization of a p-n junction in a single layer boron-phosphide. <i>Physical Chemistry Chemical Physics</i> , 2015, 17, 13013-13020.	1.3	112
11	Anisotropic exciton Stark shift in black phosphorus. <i>Physical Review B</i> , 2015, 91, .	1.1	92
12	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
13	Half-Metallic Silicon Nanowires: First-Principles Calculations. <i>Physical Review Letters</i> , 2007, 99, 256806.	2.9	70
14	Doping of rhenium disulfide monolayers: a systematic first principles study. <i>Physical Chemistry Chemical Physics</i> , 2014, 16, 16771-16779.	1.3	62
15	Comprehensive Study of Lithium Adsorption and Diffusion on Janus Mo/WXY (X, Y = S, Se, Te) Using First-Principles and Machine Learning Approaches. <i>ACS Applied Materials & Interfaces</i> , 2021, 13, 36388-36406.	4.0	52
16	Peculiar Piezoelectric Properties of Soft Two-Dimensional Materials. <i>Journal of Physical Chemistry C</i> , 2016, 120, 13948-13953.	1.5	50
17	Dependence of the electronic and transport properties of metal-MoSe ₂ /metal-MnS ₂ on contact structures. <i>Physical Review B</i> , 2014, 89, .	1.1	48
18	Fermi level pinning by integer charge transfer at electrode-organic semiconductor interfaces. <i>Applied Physics Letters</i> , 2011, 98, 113303.	1.5	42

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19	Adsorption of Pt and Bimetallic PtAu Clusters on the Partially Reduced Rutile (110) TiO ₂ Surface: A First-Principles Study. Journal of Physical Chemistry C, 2012, 116, 5735-5746.	1.5	40
20	Magnetic Properties of bcc-Fe(001)/C ₆₀ Interfaces for Organic Spintronics. ACS Applied Materials & Interfaces, 2013, 5, 837-841.	4.0	39
21	Piezoelectricity in two-dimensional materials: Comparative study between lattice dynamics and <i>ab initio</i> calculations. Physical Review B, 2017, 95, .	1.1	36
22	A distinct correlation between the vibrational and thermal transport properties of group VA monolayer crystals. Nanoscale, 2018, 10, 7803-7812.	2.8	35
23	Strain-Induced Spintronics: Modulating Electronic and Magnetic Properties of Hf ₂ MnCO ₂ MXene by Uniaxial Strain. Journal of Physical Chemistry C, 2019, 123, 12451-12459.	1.5	35
24	A systematical <i>ab-initio</i> review of promising 2D MXene monolayers towards Li-ion battery applications. JPhys Energy, 2020, 2, 032006.	2.3	34
25	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
26	Role of intrinsic molecular dipole in energy level alignment at organic interfaces. Applied Physics Letters, 2013, 102, 223301.	1.5	28
27	Modeling charge transfer at organic donor-acceptor semiconductor interfaces. Applied Physics Letters, 2012, 100, 203302.	1.5	27
28	<i>Ab initio</i> study of neutral (TiO ₂) _n clusters and their interactions with water and transition metal atoms. Journal of Physics Condensed Matter, 2012, 24, 305301.	0.7	27
29	Strain enhancement of acoustic phonon limited mobility in monolayer TiS ₃ . Physical Chemistry Chemical Physics, 2016, 18, 14434-14441.	1.3	27
30	Intercalation of Si between MoS ₂ layers. Beilstein Journal of Nanotechnology, 2017, 8, 1952-1960.	1.5	27
31	First principles study of electronic and mechanical properties of molybdenum selenide type nanowires. Physical Review B, 2006, 74, .	1.1	26
32	Dye adsorbates BrPDI, BrGly, and BrAsp on anataseTiO ₂ (001)for dye-sensitized solar cell applications. Physical Review B, 2009, 80, .	1.1	25
33	Engineering electronic properties of metal-MoSe ₂ interfaces using self-assembled monolayers. Journal of Materials Chemistry C, 2014, 2, 9842-9849.	2.7	25
34	Strain engineering of electronic and magnetic properties of double-transition metal ferromagnetic semiconductor MXenes. Journal of Applied Physics, 2019, 125, .	1.1	22
35	Assessment of Sulfur-Functionalized MXenes for Li-Ion Battery Applications. Journal of Physical Chemistry C, 2020, 124, 21293-21304.	1.5	22
36	First-principles study of thin TiO_2 bulklike rutile nanowires. Physical Review B, 2009, 80, .	1.1	21

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37	Charge equilibration and potential steps in organic semiconductor multilayers. <i>Organic Electronics</i> , 2012, 13, 1793-1801.	1.4	21
38	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
39	Magnetoresistance in multilayer fullerene spin valves: A first-principles study. <i>Physical Review B</i> , 2014, 90, .	1.1	20
40	Achieving Fast Kinetics and Enhanced Li Storage Capacity for Ti ₃ C ₂ O ₂ by Intercalation of Quinone Molecules. <i>ACS Applied Energy Materials</i> , 2019, 2, 1251-1258.	2.5	19
41	Gate induced monolayer behavior in twisted bilayer black phosphorus. <i>2D Materials</i> , 2017, 4, 035025.	2.0	18
42	Determination of Dynamically Stable Electrenes toward Ultrafast Charging Battery Applications. <i>Journal of Physical Chemistry Letters</i> , 2018, 9, 4267-4274.	2.1	18
43	Tailoring Storage Capacity and Ion Kinetics in Ti ₂ CO ₂ / Graphene Heterostructures by Functionalization of Graphene. <i>Physical Review Applied</i> , 2019, 12, .	1.5	17
44	From spin-polarized interfaces to giant magnetoresistance in organic spin valves. <i>Physical Review B</i> , 2014, 89, .	1.1	15
45	Revealing the Formation Energyâ€“Exfoliation Energyâ€“Structure Correlation of MAB Phases Using Machine Learning and DFT. <i>ACS Applied Materials & Interfaces</i> , 2020, 12, 29424-29431.	4.0	15
46	Coal-Derived Graphene/MoS ₂ Heterostructure Electrodes for Li-Ion Batteries: Experiment and Simulation Study. <i>ACS Applied Materials & Interfaces</i> , 2021, 13, 59950-59961.	4.0	15
47	Native Defects and the Dehydrogenation of NaBH ₄ . <i>Journal of Physical Chemistry C</i> , 2011, 115, 24429-24434.	1.5	13
48	On the structural and electronic properties of Ir-silicide nanowires on Si(001) surface. <i>Journal of Applied Physics</i> , 2016, 120, .	1.1	8
49	Electronic and mechanical properties of stiff rhenium carbide monolayers: A first-principles investigation. <i>Applied Surface Science</i> , 2018, 458, 762-768.	3.1	8
50	Stability of adsorption of Mg and Na on sulfur-functionalized MXenes. <i>Physical Chemistry Chemical Physics</i> , 2021, 23, 25424-25433.	1.3	8
51	Interaction of BrPDI, BrGly, and BrAsp with the Rutile 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
52	Fluorographane: a promising material for bipolar doping of MoS ₂ . <i>Physical Chemistry Chemical Physics</i> , 2015, 17, 27636-27641.	1.3	7
53	In pursuit of barrierless transition metal dichalcogenides lateral heterojunctions. <i>Nanotechnology</i> , 2018, 29, 295202.	1.3	6
54	First-principles discovery of stable two-dimensional materials with high-level piezoelectric response. <i>Journal of Physics Condensed Matter</i> , 2021, 33, 115705.	0.7	5

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55	Scanning Tunneling Microscopy and Density Functional Theory Study on Zinc(II)-Phthalocyanine Tetrasulfonic Acid on Bilayer Epitaxial Graphene on Silicon Carbide(0001). Journal of Physical Chemistry C, 2015, 119, 9845-9850.	1.5	4
56	Enhanced Electrochemical Storage Properties of Na- and Mg-Intercalated B-Doped-Graphene Based Heterostructures and Bilayers. Journal of Physical Chemistry C, 2020, 124, 1260-1268.	1.5	4
57	Angle-resolved synchrotron photoemission and density functional theory on the iridium modified Si(111) surface. Journal of Physics Condensed Matter, 2014, 26, 285501.	0.7	3
58	Silicene-Like Domains on IrSi ₃ Crystallites. Journal of Physical Chemistry C, 2019, 123, 7225-7229.	1.5	3
59	Engineering magnetic anisotropy and exchange couplings in double transition metal MXenes via surface defects. Journal of Physics Condensed Matter, 2021, 33, 035801.	0.7	2
60	Study of iridium silicide monolayers using density functional theory. Journal of Applied Physics, 2018, 123, 074301.	1.1	1