Deniz Cakir

List of Publications by Year
in descending order

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Version: 2024-02-01

60 papers	2,983 citations	201674 27 h-index	161849 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. Physical Review B, 2014, 90, .	3.2	279
2	Mo₂C as a high capacity anode material: a first-principles study. Journal of Materials Chemistry A, 2016, 4, 6029-6035.	10.3	249
3	MXenes/graphene heterostructures for Li battery applications: a first principles study. Journal of Materials Chemistry A, 2018, 6, 2337-2345.	10.3	173
4	Promising Piezoelectric Performance of Single Layer Transition-Metal Dichalcogenides and Dioxides. Journal of Physical Chemistry C, 2015, 119, 23231-23237.	3.1	164
5	Mechanical and thermal properties of h-MX₂ (Mâ€‰=â€‰Cr, Mo, W; Xâ€‰=â€‰O, S, Se, Te) monolayers: A comparative study. Applied Physics Letters, 2014, 104, 203110.	3.3	157
6	Significant effect of stacking on the electronic and optical properties of few-layer black phosphorus. Physical Review B, 2015, 92, .	3.2	152
7	Formation and stability of point defects in monolayer rhenium disulfide. Physical Review B, 2014, 89, .	3.2	151
8	Thermal properties of black and blue phosphorenes from a first-principles quasiharmonic approach. Physical Review B, 2015, 92, .	3.2	140
9	The influence of surface functionalization on thermal transport and thermoelectric properties of MXene monolayers. Nanoscale, 2018, 10, 8859-8868.	5.6	118
10	Realization of a pâ€“n junction in a single layer boron-phosphide. Physical Chemistry Chemical Physics, 2015, 17, 13013-13020.	2.8	112
11	Anisotropic exciton Stark shift in black phosphorus. Physical Review B, 2015, 91, .	3.2	92
12	Alkali Metal Intercalation in MXene/Graphene Heterostructures: A New Platform for Ion Battery Applications. Journal of Physical Chemistry Letters, 2019, 10, 727-734.	4.6	88
13	Half-Metallic Silicon Nanowires: First-Principles Calculations. Physical Review Letters, 2007, 99, 256806.	7.8	70
14	Doping of rhenium disulfide monolayers: a systematic first principles study. Physical Chemistry Chemical Physics, 2014, 16, 16771-16779.	2.8	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. ACS Applied Materials & Interfaces, 2021, 13, 36388-36406.	8.0	52
16	Peculiar Piezoelectric Properties of Soft Two-Dimensional Materials. Journal of Physical Chemistry C, 2016, 120, 13948-13953.	3.1	50
17	Dependence of the electronic and transport properties of<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mtext>metal-MoSe</mml:mtext><mml:mn>2</mml:mn></mml:msub></mml:math> on contact structures. Physical Review B, 2014, 89, .	3.2	48
18	Fermi level pinning by integer charge transfer at electrode-organic semiconductor interfaces. Applied Physics Letters, 2011, 98, 113303.	3.3	42

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19	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.	3.1	40
20	Magnetic Properties of bcc-Fe(001)/C₆₀ Interfaces for Organic Spintronics. ACS Applied Materials & Interfaces, 2013, 5, 837-841.	8.0	39
21	Piezoelectricity in two-dimensional materials: Comparative study between lattice dynamics andab initiocalculations. Physical Review B, 2017, 95, .	3.2	36
22	A distinct correlation between the vibrational and thermal transport properties of group VA monolayer crystals. Nanoscale, 2018, 10, 7803-7812.	5.6	35
23	Strainâ€“Spintronics: Modulating Electronic and Magnetic Properties of Hf₂MnC₂O₂ MXene by Uniaxial Strain. Journal of Physical Chemistry C, 2019, 123, 12451-12459.	3.1	35
24	A systematical ab-initio review of promising 2D MXene monolayers towards Li-ion battery applications. JPhys Energy, 2020, 2, 032006.	5.3	34
25	Effect of impurities on the mechanical and electronic properties of Au, Ag, and Cu monatomic chain nanowires. Physical Review B, 2011, 84, .	3.2	30
26	Role of intrinsic molecular dipole in energy level alignment at organic interfaces. Applied Physics Letters, 2013, 102, 223301.	3.3	28
27	Modeling charge transfer at organic donor-acceptor semiconductor interfaces. Applied Physics Letters, 2012, 100, 203302.	3.3	27
28	Ab initiostudy of neutral (TiO₂)_nclusters and their interactions with water and transition metal atoms. Journal of Physics Condensed Matter, 2012, 24, 305301.	1.8	27
29	Strain enhancement of acoustic phonon limited mobility in monolayer TiS₃. Physical Chemistry Chemical Physics, 2016, 18, 14434-14441.	2.8	27
30	Intercalation of Si between MoS₂ layers. Beilstein Journal of Nanotechnology, 2017, 8, 1952-1960.	2.8	27
31	First principles study of electronic and mechanical properties of molybdenum selenide type nanowires. Physical Review B, 2006, 74, .	3.2	26
32	Dye adsorbates BrPDI, BrGly, and BrAsp on anataseTiO2(001)for dye-sensitized solar cell applications. Physical Review B, 2009, 80, .	3.2	25
33	Engineering electronic properties of metalâ€“MoSe₂ interfaces using self-assembled monolayers. Journal of Materials Chemistry C, 2014, 2, 9842-9849.	5.5	25
34	Strain engineering of electronic and magnetic properties of double-transition metal ferromagnetic semiconductor MXenes. Journal of Applied Physics, 2019, 125, .	2.5	22
35	Assessment of Sulfur-Functionalized MXenes for Li-Ion Battery Applications. Journal of Physical Chemistry C, 2020, 124, 21293-21304.	3.1	22
36	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, .	3.2	21

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37	Charge equilibration and potential steps in organic semiconductor multilayers. Organic Electronics, 2012, 13, 1793-1801.	2.6	21
38	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, .	3.2	21
39	Magnetoresistance in multilayer fullerene spin valves: A first-principles study. Physical Review B, 2014, 90, .	3.2	20
40	Achieving Fast Kinetics and Enhanced Li Storage Capacity for Ti3C2O2 by Intercalation of Quinone Molecules. ACS Applied Energy Materials, 2019, 2, 1251-1258.	5.1	19
41	Gate induced monolayer behavior in twisted bilayer black phosphorus. 2D Materials, 2017, 4, 035025.	4.4	18
42	Determination of Dynamically Stable Electrenes toward Ultrafast Charging Battery Applications. Journal of Physical Chemistry Letters, 2018, 9, 4267-4274.	4.6	18
43	Tailoring Storage Capacity and Ion Kinetics in Ti2CO2/ Graphene Heterostructures by Functionalization of Graphene. Physical Review Applied, 2019, 12, .	3.8	17
44	From spin-polarized interfaces to giant magnetoresistance in organic spin valves. Physical Review B, 2014, 89, .	3.2	15
45	Revealing the Formation Energyâ€“Exfoliation Energyâ€“Structure Correlation of MAB Phases Using Machine Learning and DFT. ACS Applied Materials & Interfaces, 2020, 12, 29424-29431.	8.0	15
46	Coal-Derived Graphene/MoS₂ Heterostructure Electrodes for Li-Ion Batteries: Experiment and Simulation Study. ACS Applied Materials & Interfaces, 2021, 13, 59950-59961.	8.0	15
47	Native Defects and the Dehydrogenation of NaBH4. Journal of Physical Chemistry C, 2011, 115, 24429-24434.	3.1	13
48	On the structural and electronic properties of Ir-silicide nanowires on Si(001) surface. Journal of Applied Physics, 2016, 120, .	2.5	8
49	Electronic and mechanical properties of stiff rhenium carbide monolayers: A first-principles investigation. Applied Surface Science, 2018, 458, 762-768.	6.1	8
50	Stability of adsorption of Mg and Na on sulfur-functionalized MXenes. Physical Chemistry Chemical Physics, 2021, 23, 25424-25433.	2.8	8
51	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.	3.1	7
52	Fluorographane: a promising material for bipolar doping of MoS2. Physical Chemistry Chemical Physics, 2015, 17, 27636-27641.	2.8	7
53	In pursuit of barrierless transition metal dichalcogenides lateral heterojunctions. Nanotechnology, 2018, 29, 295202.	2.6	6
54	First-principles discovery of stable two-dimensional materials with high-level piezoelectric response. Journal of Physics Condensed Matter, 2021, 33, 115705.	1.8	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.	3.1	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.	3.1	4
57	Angle-resolved synchrotron photoemission and density functional theory on the iridium modified Si(1â€‰1â€‰1) surface. Journal of Physics Condensed Matter, 2014, 26, 285501.	1.8	3
58	Silicene-Like Domains on IrSi₃ Crystallites. Journal of Physical Chemistry C, 2019, 123, 7225-7229.	3.1	3
59	Engineering magnetic anisotropy and exchange couplings in double transition metal MXenes via surface defects. Journal of Physics Condensed Matter, 2021, 33, 035801.	1.8	2
60	Study of iridium silicide monolayers using density functional theory. Journal of Applied Physics, 2018, 123, 074301.	2.5	1