Deniz Cakir

List of Publications by Year in Descending Order

58 papers	2,255 citations	24 h-index	47 g-index
60 ext. papers	2,617 ext. citations	4.5 avg, IF	5.54 L-index

#	Paper	IF	Citations
58	Stability of adsorption of Mg and Na on sulfur-functionalized MXenes. *Physical Chemistry Chemical Physics*, **2021**, 23, 25424-25433	3.6	2
57	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	9.5	12
56	Revealing the Formation Energy-Exfoliation Energy-Structure Correlation of MAB Phases Using Machine Learning and DFT. *ACS Applied Materials & Interfaces*, **2020**, 12, 29424-29431	9.5	7
55	Engineering magnetic anisotropy and exchange couplings in double transition metal MXenes via surface defects. *Journal of Physics Condensed Matter*, **2020**, 33, 035801	1.8	1
54	A systematical ab-initio review of promising 2D MXene monolayers towards Li-ion battery applications. *JPhys Energy*, **2020**, 2, 032006	4.9	14
53	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	3.8	4
52	Assessment of Sulfur-Functionalized MXenes for Li-Ion Battery Applications. *Journal of Physical Chemistry C*, **2020**, 124, 21293-21304	3.8	8
51	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
50	Strain Spintronics: Modulating Electronic and Magnetic Properties of Hf2MnC2O2 MXene by Uniaxial Strain. *Journal of Physical Chemistry C*, **2019**, 123, 12451-12459	3.8	19
49	Silicene-Like Domains on IrSi3 Crystallites. *Journal of Physical Chemistry C*, **2019**, 123, 7225-7229	3.8	3
48	Tailoring Storage Capacity and Ion Kinetics in Ti2CO2/Graphene Heterostructures by Functionalization of Graphene. *Physical Review Applied*, **2019**, 12,	4.3	14
47	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
46	Achieving Fast Kinetics and Enhanced Li Storage Capacity for Ti3C2O2 by Intercalation of Quinone Molecules. *ACS Applied Energy Materials*, **2019**, 2, 1251-1258	6.1	15
45	Strain engineering of electronic and magnetic properties of double-transition metal ferromagnetic semiconductor MXenes. *Journal of Applied Physics*, **2019**, 125, 082527	2.5	12
44	The influence of surface functionalization on thermal transport and thermoelectric properties of MXene monolayers. *Nanoscale*, **2018**, 10, 8859-8868	7.7	72
43	Study of iridium silicide monolayers using density functional theory. *Journal of Applied Physics*, **2018**, 123, 074301	2.5	0
42	MXenes/graphene heterostructures for Li battery applications: a first principles study. *Journal of Materials Chemistry A*, **2018**, 6, 2337-2345	13	119

41	In pursuit of barrierless transition metal dichalcogenides lateral heterojunctions. *Nanotechnology*, **2018**, 29, 295202	3.4	3
40	A distinct correlation between the vibrational and thermal transport properties of group VA monolayer crystals. *Nanoscale*, **2018**, 10, 7803-7812	7.7	23
39	Electronic and mechanical properties of stiff rhenium carbide monolayers: A first-principles investigation. *Applied Surface Science*, **2018**, 458, 762-768	6.7	4
38	Determination of Dynamically Stable Electrenes toward Ultrafast Charging Battery Applications. *Journal of Physical Chemistry Letters*, **2018**, 9, 4267-4274	6.4	7
37	Piezoelectricity in two-dimensional materials: Comparative study between lattice dynamics and ab initio calculations. *Physical Review B*, **2017**, 95,	3.3	25
36	Gate induced monolayer behavior in twisted bilayer black phosphorus. *2D Materials*, **2017**, 4, 035025	5.9	12
35	Intercalation of Si between MoS layers. *Beilstein Journal of Nanotechnology*, **2017**, 8, 1952-1960	3	20
34	Strain enhancement of acoustic phonon limited mobility in monolayer TiS3. *Physical Chemistry Chemical Physics*, **2016**, 18, 14434-41	3.6	24
33	Peculiar Piezoelectric Properties of Soft Two-Dimensional Materials. *Journal of Physical Chemistry C* , **2016**, 120, 13948-13953	3.8	32
32	Mo2C as a high capacity anode material: a first-principles study. *Journal of Materials Chemistry A*, **2016**, 4, 6029-6035	13	179
31	On the structural and electronic properties of Ir-silicide nanowires on Si(001) surface. *Journal of Applied Physics*, **2016**, 120, 095303	2.5	8
30	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	3.8	4
29	Realization of a p-n junction in a single layer boron-phosphide. *Physical Chemistry Chemical Physics*, **2015**, 17, 13013-20	3.6	93
28	Fluorographane: a promising material for bipolar doping of MoS2. *Physical Chemistry Chemical Physics*, **2015**, 17, 27636-41	3.6	7
27	Promising Piezoelectric Performance of Single Layer Transition-Metal Dichalcogenides and Dioxides. *Journal of Physical Chemistry C*, **2015**, 119, 23231-23237	3.8	114
26	Thermal properties of black and blue phosphorenes from a first-principles quasiharmonic approach. *Physical Review B*, **2015**, 92,	3.3	111
25	Significant effect of stacking on the electronic and optical properties of few-layer black phosphorus. *Physical Review B*, **2015**, 92,	3.3	135
24	Anisotropic exciton Stark shift in black phosphorus. *Physical Review B*, **2015**, 91,	3.3	85

23	Tuning of the electronic and optical properties of single-layer black phosphorus by strain. *Physical Review B*, **2014**, 90,	3.3	235
22	Doping of rhenium disulfide monolayers: a systematic first principles study. *Physical Chemistry Chemical Physics*, **2014**, 16, 16771-9	3.6	56
21	Angle-resolved synchrotron photoemission and density functional theory on the iridium modified Si(1 1 1) surface. *Journal of Physics Condensed Matter*, **2014**, 26, 285501	1.8	3
20	From spin-polarized interfaces to giant magnetoresistance in organic spin valves. *Physical Review B*, **2014**, 89,	3.3	14
19	Mechanical and thermal properties of h-MX2 (M = Cr, Mo, W; X = O, S, Se, Te) monolayers: A comparative study. *Applied Physics Letters*, **2014**, 104, 203110	3.4	110
18	Dependence of the electronic and transport properties of metal-MoSe2 interfaces on contact structures. *Physical Review B*, **2014**, 89,	3.3	38
17	Engineering electronic properties of metal MoSe2 interfaces using self-assembled monolayers. *Journal of Materials Chemistry C*, **2014**, 2, 9842-9849	7.1	21
16	Formation and stability of point defects in monolayer rhenium disulfide. *Physical Review B*, **2014**, 89,	3.3	118
15	Magnetoresistance in multilayer fullerene spin valves: A first-principles study. *Physical Review B*, **2014**, 90,	3.3	18
14	Magnetic properties of bcc-Fe(001)/C interfaces for organic spintronics. *ACS Applied Materials & Interfaces*, **2013**, 5, 837-41	9.5	33
13	Role of intrinsic molecular dipole in energy level alignment at organic interfaces. *Applied Physics Letters*, **2013**, 102, 223301	3.4	25
12	Modeling charge transfer at organic donor-acceptor semiconductor interfaces. *Applied Physics Letters*, **2012**, 100, 203302	3.4	25
11	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
10	Charge equilibration and potential steps in organic semiconductor multilayers. *Organic Electronics*, **2012**, 13, 1793-1801	3.5	19
9	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
8	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
7	Native Defects and the Dehydrogenation of NaBH4. *Journal of Physical Chemistry C*, **2011**, 115, 24429-24484	3.8	12
6	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

5	Fermi level pinning by integer charge transfer at electrode-organic semiconductor interfaces. *Applied Physics Letters*, **2011**, 98, 113303	3.4	41
4	Dye adsorbates BrPDI, BrGly, and BrAsp on anatase TiO2(001) for dye-sensitized solar cell applications. *Physical Review B*, **2009**, 80,	3.3	25
3	First-principles study of thin TiOx and bulklike rutile nanowires. *Physical Review B*, **2009**, 80,	3.3	21
2	Half-metallic silicon nanowires: first-principles calculations. *Physical Review Letters*, **2007**, 99, 256806	7.4	66
1	First principles study of electronic and mechanical properties of molybdenum selenide type nanowires. *Physical Review B*, **2006**, 74,	3.3	21