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List of Publications by Year in descending order

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#	ARTICLE	IF	CITATIONS
1	Elucidating the Barriers on Direct Water Splitting: Key Role of Oxygen Vacancy Density and Coordination over PbTiO ₃ and TiO ₂ . Journal of Physical Chemistry C, 2021, 125, 1874-1880.	3.1	5
2	Mechanism of transition metal interaction with graphene sheet reflected in its plasmonic excitations: Effect of gas adsorption phenomena studied by a combination of solid state and molecular orbital approaches. Applied Surface Science, 2021, 554, 149585.	6.1	1
3	Double Perovskite Structure Induced by Co Addition to PbTiO ₃ : Insights from DFT and Experimental Solid-State NMR Spectroscopy. Journal of Physical Chemistry C, 2019, 123, 27132-27139.	3.1	8
4	DFT Characterization of Metallolite-Decorated Silicon (001) Surface. Journal of Physical Chemistry C, 2019, 123, 11639-11648.	3.1	0
5	Alkali and Alkaline earth metal doped aluminum tetraborides containing intrinsic planar boron sheet: XAlB ₄ (X= Li, Mg, Ca, and Na). Computational Materials Science, 2016, 124, 130-141.	3.0	5
6	Structural and electronic properties of AB- and AA-stacking bilayer-graphene intercalated by Li, Na, Ca, B, Al, Si, Ge, Ag, and Au atoms. Solid State Communications, 2016, 231-232, 57-63.	1.9	15
7	Anatase TiO ₂ nanowires functionalized by organic sensitizers for solar cells: A screened Coulomb hybrid density functional study. Journal of Applied Physics, 2015, 118, 194301.	2.5	5
8	Hybrid functional calculated optical and electronic structures of thin anatase TiO ₂ nanowires with organic dye adsorbates. Applied Surface Science, 2015, 354, 437-442.	6.1	3
9	Theoretical investigation of charge accumulation layer on the Bi-induced InAs(111)-(2×2) surface. Journal of Applied Physics, 2014, 115, 163702.	2.5	0
10	Range-Separated Hybrid Density Functional Study of Organic Dye Sensitizers on Anatase TiO ₂ Nanowires. Journal of Physical Chemistry C, 2014, 118, 24776-24783.	3.1	2
11	Electronic structures and optical spectra of thin anatase TiO ₂ nanowires through hybrid density functional and quasiparticle calculations. Physical Review B, 2014, 89, .	3.1	2
12	Influence of Steps on the Tilting and Adsorption Dynamics of Ordered Pentacene Films on Vicinal Ag(111) Surfaces. Journal of Physical Chemistry C, 2012, 116, 19429-19433.	3.1	13
13	Interaction of BrPDI, BrGly, and BrAsp with the Rutile TiO ₂ (110) Surface for Photovoltaic and Photocatalytic Applications: A First-Principles Study. Journal of Physical Chemistry C, 2011, 115, 9220-9226.	3.1	7
14	Electronic and structural properties of armchair SWCNT/TiO ₂ (110)-(1×2) system. Surface Science, 2011, 605, 593-596.	1.9	2
15	Electronic structure and excess charge in (1×2) TiO ₂ (110) from DFT	3.2	11
16	Theoretical analysis of small Pt particles on rutileTiO ₂ (110)surfaces. Physical Review B, 2010, 82, .	3.2	38
17	Pentacene Multilayers on Ag(111) Surface. Journal of Physical Chemistry C, 2010, 114, 2724-2729.	3.1	28
18	Dye adsorbates BrPDI, BrGly, and BrAsp on anataseTiO ₂ (001)for dye-sensitized solar cell applications. Physical Review B, 2009, 80, .	3.2	25

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19	Modification of TiO_2 electronic structure by Au impurity investigated with density functional theory. Physical Review B, 2009, 80, .	3.2	16
20	Atomic and electronic structure of group-IV adsorbates on the GaAs(001)-(1Å–2) surface. Surface Science, 2009, 603, 2683-2687.	1.9	3
21	Pt-incorporated anatase TiO_2 for solar cell applications: First-principles density functional theory calculations. Physical Review B, 2009, 79, .	3.2	28
22	Atomic and electronic structure of Bi/GaAs(001)- $\hat{1}\pm 2(2 \text{ \AA} - 4)$. Journal of Physics Condensed Matter, 2008, 20, 265003.	1.8	6
23	Chemisorption of 3-Aminopropyltrimethoxysilane on Si(001)-(2 Å– 2). Journal of Physical Chemistry C, 2007, 111, 15020-15025.	3.1	10
24	An ab initio study of 3-aminopropyltrimethoxysilane molecule on Si(111)-() surface. Surface Science, 2007, 601, 3740-3744.	1.9	10
25	Effect of hydrogenation on B/Si(001)-(1Å–2). Surface Science, 2007, 601, 3711-3716.	1.9	2
26	Atomic and electronic structure of Sr/Si(001)-(2Å–2). Surface Science, 2006, 600, 3614-3618.	1.9	5
27	Lattice vibrations of pure and doped GaSe. Materials Research Bulletin, 2006, 41, 751-763.	5.2	52
28	DFT study of Rb/Si(100)-2Å–1 system. Surface Science, 2005, 583, 119-125.	1.9	3
29	Cs adsorption on Si(001) surface: Anab initiostudy. Physical Review B, 2005, 72, .	3.2	12
30	Mg adsorption on Si(001) surface from first principles. Physical Review B, 2004, 69, .	3.2	11
31	An ab initio study of the Te surfactant on Ge/Si(001). Surface Science, 2004, 566-568, 719-722.	1.9	1
32	Ab initio study of the one-monolayer Sb/Ge interface. Surface Science, 2004, 566-568, 956-960.	1.9	3
33	Electronic structure of the chainlike compound TlSe. Physical Review B, 2004, 70, .	3.2	31
34	Ab initio study of the one-monolayer Sb/Si(001) interface. Surface Science, 2003, 532-535, 661-665.	1.9	5
35	Electronic and structural properties of a4dperovskite: Cubic phase ofSrZrO3. Physical Review B, 2003, 68, .	3.2	96
36	Adsorption of Te on Ge(001): Density-functional calculations. Physical Review B, 2003, 67, .	3.2	5

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37	Spatial stabilization of Townsend and glow discharges with a semiconducting cathode. Journal Physics D: Applied Physics, 1996, 29, 628-633.	2.8	31
38	Low-temperature second harmonic generation in gallium selenide under resonant excitation of the direct free excitons. Solid State Communications, 1995, 93, 147-150.	1.9	9
39	Chemisorption of a p-adsorbate on perovskites. Physica B: Condensed Matter, 1994, 193, 39-44.	2.7	0
40	Raman scattering and Hall effect in layer InSe under pressure. High Pressure Research, 1994, 13, 121-125.	1.2	2
41	Raman scattering in layer indium selenide under pressure. Solid State Communications, 1993, 87, 675-678.	1.9	14
42	Low-temperature phase transitions in TlGaS ₂ layer crystals. Solid State Communications, 1993, 88, 387-390.	1.9	18
43	Elastic coefficients in TlGa(S _{1-x} Se _x) ₂ and TlIn _x Ga _{1-x} S ₂ layer mixed crystal by Brillouin scattering. Physica B: Condensed Matter, 1993, 192, 371-377.	2.7	11
44	Elastic Properties of GaS _{1-x} Se _x Layer Mixed Crystals by Brillouin Scattering. Physica Status Solidi (B): Basic Research, 1993, 177, K59.	1.5	1
45	Electronic structure of strained Si _n /Ge _n (001) superlattices. Solid State Communications, 1988, 65, 1285-1290.	1.9	9
46	Calculations of STM linescans - general formalism. Solid State Communications, 1988, 66, 1135-1139.	1.9	2
47	Density-of-states and partial-density-of-states functions for the cubicd-band perovskites. Physical Review B, 1982, 25, 2697-2714.	3.2	33
48	Interpretation of the spectra obtained from oxygen-adsorbed and oxidized silicon surfaces. Physical Review B, 1982, 26, 5716-5729.	3.2	70
49	An investigation of the interface electronics structure of Siâ€“SiO ₂ junctions. Journal of Vacuum Science and Technology, 1982, 21, 402-404.	1.9	3
50	Chemisorption of atomic oxygen on silicon surface. Solid State Communications, 1982, 42, 879-881.	1.9	7
51	Matrix element effects in 2 % of the insulating perovskites. Applied Physics Berlin, 1980, 22, 11-13.	1.4	2
52	Neutron Scattering by Magnons of an Antiferromagnet with Modulated Spin Amplitudes. Physical Review Letters, 1980, 44, 1295-1298.	7.8	17
53	Model for the x-ray photoelectron distributions of d-band perovskites. Physical Review B, 1979, 19, 43-46.	3.2	14
54	Surface states on n-type SrTiO ₃ . Solid State Communications, 1978, 27, 321-324.	1.9	23

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55	Surface electronic properties of d-band perovskites: Study of the ϵ -bands. Physical Review B, 1978, 18, 4509-4525.	3.2	37
56	Surface enhanced covalency and its effect on the surface states of d-band metal oxides. Applied Physics Berlin, 1977, 13, 21-24.	1.4	29