Jorge O Sofo

List of Publications by Year
in descending order

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95 papers	9,280 citations	87723 38 h-index	48187 88 g-index
98 all docs	98 docs citations	98 times ranked	10402 citing authors

#	Article	IF	Citations
1	Graphane: A two-dimensional hydrocarbon. Physical Review B, 2007, 75, .	1.1	1,744
2	The best thermoelectric.. Proceedings of the National Academy of Sciences of the United States of America, 1996, 93, 7436-7439.	3.3	1,385
3	Linear optical properties of solids within the full-potential linearized augmented planewave method. Computer Physics Communications, 2006, 175, 1-14.	3.0	1,215
4	Transport coefficients from first-principles calculations. Physical Review B, 2003, 68, .	1.1	663
5	Reversible fluorination of graphene: Evidence of a two-dimensional wide bandgap semiconductor. Physical Review B, 2010, 81, .	1.1	365
6	First-principles study of binary bcc alloys using special quasirandom structures. Physical Review B, 2004, 69, .	1.1	266
7	n-Type Behavior of Graphene Supported on Si/SiO₂ Substrates. ACS Nano, 2008, 2, 2037-2044.	7.3	241
8	Optimum band gap of a thermoelectric material. Physical Review B, 1994, 49, 4565-4570.	1.1	221
9	Electronic structure ofCoSb3:A narrow-band-gap semiconductor. Physical Review B, 1998, 58, 15620-15623.	1.1	179
10	Thermoelectric properties ofSb2Te3under pressure and uniaxial stress. Physical Review B, 2003, 68, .	1.1	175
11	Thermoelectric figure of merit of superlattices. Applied Physics Letters, 1994, 65, 2690-2692.	1.5	167
12	Multilayer thermionic refrigerator and generator. Journal of Applied Physics, 1998, 83, 4683-4689.	1.1	148
13	Scanning Tunneling Microscopy Chemical Signature of Point Defects on theMoS2(0001)Surface. Physical Review Letters, 2004, 92, 026802.	2.9	105
14	Gate-Voltage Control of Oxygen Diffusion on Graphene. Physical Review Letters, 2011, 106, 146802.	2.9	99
15	Development of a ReaxFF Reactive Force Field for Titanium Dioxide/Water Systems. Langmuir, 2013, 29, 7838-7846.	1.6	96
16	Surface Protonation at the Rutile (110) Interface: Explicit Incorporation of Solvation Structure within the Refined MUSIC Model Framework. Langmuir, 2008, 24, 12331-12339.	1.6	88
17	Electronic structure of the pyrochlore metalsCd2Os2O7andCd2Re2O7. Physical Review B, 2002, 65, .	1.1	81
18	Comparisons of Multilayer H₂O Adsorption onto the (110) Surfaces of Î±-TiO₂ and SnO₂ as Calculated with Density Functional Theory. Journal of Physical Chemistry B, 2008, 112, 11616-11624.	1.2	81

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19	Oxygen migration on the graphene surface. 2. Thermochemistry of basal-plane diffusion (hopping). Carbon, 2011, 49, 4226-4238.	5.4	78
20	Stress-induced defects inSb2Te3. Physical Review B, 2003, 68, .	1.1	77
21	Electrical control of the chemical bonding of fluorine on graphene. Physical Review B, 2011, 83, .	1.1	76
22	Hydrogen Bonds and Vibrations of Water on (110) Rutile. Journal of Physical Chemistry C, 2009, 113, 13732-13740.	1.5	74
23	Van der Waals Dispersion Forces between Dielectric Nanoclusters. Langmuir, 2007, 23, 1735-1740.	1.6	73
24	Periodic Density Functional Theory Study of Water Adsorption on the Î±-Quartz (101) Surface. Journal of Physical Chemistry C, 2011, 115, 5756-5766.	1.5	73
25	Calculation of the electronic and structural properties of cubicMg2NiH4. Physical Review B, 1999, 59, 11746-11754.	1.1	63
26	van der Waals forces between nanoclusters: Importance of many-body effects. Journal of Chemical Physics, 2006, 124, 074504.	1.2	57
27	Derivation of Force Field Parameters for SnO2â^'H2O Surface Systems from Plane-Wave Density Functional Theory Calculations. Journal of Physical Chemistry B, 2006, 110, 8386-8397.	1.2	53
28	Structure of hydrated Zn2+ at the rutile TiO2 (110)-aqueous solution interface: Comparison of X-ray standing wave, X-ray absorption spectroscopy, and density functional theory results. Geochimica Et Cosmochimica Acta, 2006, 70, 4039-4056.	1.6	52
29	A New Hypothesis for the Dissolution Mechanism of Silicates. Journal of Physical Chemistry C, 2012, 116, 17479-17491.	1.5	52
30	Vibrational Density of States of Strongly H-Bonded Interfacial Water: Insights from Inelastic Neutron Scattering and Theory. Journal of Physical Chemistry C, 2014, 118, 10805-10813.	1.5	48
31	An integrated framework for multi-scale materials simulation and design. Journal of Computer-Aided Materials Design, 2004, 11, 183-199.	0.7	46
32	Static polarizabilities of dielectric nanoclusters. Physical Review A, 2005, 72, .	1.0	46
33	Comment on â€œStructure and dynamics of liquid water on rutile TiO2(110)â€• Physical Review B, 2012, 85, .	1.1	46
34	Magnetic structure of hydrogen-induced defects on graphene. Physical Review B, 2012, 85, .	1.1	46
35	Electronic structure calculations of physisorption and chemisorption on oxide glass surfaces. Physical Review B, 2005, 72, .	1.1	44
36	Linking first-principles energetics to CALPHAD: An application to thermodynamic modeling of the Al-Ca binary system. Metallurgical and Materials Transactions A: Physical Metallurgy and Materials Science, 2005, 36, 5-13.	1.1	41

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37	Thermodynamics modeling of the Mgâ€“Sr and Caâ€“Mgâ€“Sr systems. Journal of Alloys and Compounds, 2006, 421, 172-178.	2.8	41
38	Effect of Ions on H-Bond Structure and Dynamics at the Quartz(101)â€“Water Interface. Langmuir, 2016, 32, 11353-11365.	1.6	41
39	Contribution of first-principles energetics to the Caâ€“Mg thermodynamic modeling. Journal of Alloys and Compounds, 2006, 420, 98-106.	2.8	36
40	Faster proton transfer dynamics of water on SnO2 compared to TiO2. Journal of Chemical Physics, 2011, 134, 044706.	1.2	34
41	Resistivity and superconductivity from anharmonic phonons. Physical Review B, 1993, 47, 8050-8055.	1.1	33
42	Adsorption of Pd onMoS2(1000):Ab initioelectronic-structure calculations. Physical Review B, 1999, 60, 8343-8347.	1.1	32
43	Improved thermoelectric devices using bismuth alloys. Applied Physics Letters, 2004, 85, 588-590.	1.5	32
44	Intrinsic bistability in resonant-tunneling structures. Physical Review B, 1990, 42, 7292-7295.	1.1	31
45	Photoluminescence from nanocrystalline graphite monofluoride. Applied Physics Letters, 2010, 97, .	1.5	31
46	Metal-insulator transition in the double perovskites. Physical Review B, 2001, 64, .	1.1	28
47	Collective excitations in superconductors: From Bardeen-Cooper-Schrieffer theory to Bose condensation. Physical Review B, 1992, 45, 9860-9864.	1.1	26
48	Bending energy of 2D materials: graphene, MoS₂ and imogolite. RSC Advances, 2018, 8, 4577-4583.	1.7	26
49	Electrically tunable multiple Dirac cones in thin films of the (LaO)2(SbSe2)2 family of materials. Nature Communications, 2015, 6, 8517.	5.8	25
50	A density-functional study of the structural, electronic, magnetic, and vibrational properties of Ti8C12 metallocarbohedrynes. Journal of Chemical Physics, 2005, 123, 154106.	1.2	23
51	Anion Photoelectron Spectroscopy and Density Functional Investigation of Vanadium Carbide Clusters. Journal of Physical Chemistry A, 2006, 110, 12814-12821.	1.1	22
52	Metal-substituted Ti8C12 metallocarbohedrynes: toward less reactive clusters as building blocks of cluster-assembled materials. Physical Chemistry Chemical Physics, 2012, 14, 9642.	1.3	21
53	Analysis and optimization of carbon nanotubes and graphene sensors based on adsorption-desorption kinetics. Applied Physics Letters, 2013, 103, .	1.5	21
54	Density functional theory simulation of hydrogen-bonding structure and vibrational densities of states at the quartz (1â€‰0â€‰1)-water interface and its relation to dissolution as a function of solution pH and ionic strength. Journal of Physics Condensed Matter, 2014, 26, 244101.	0.7	20

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55	Impurity State and Variable Range Hopping Conduction in Graphene. Physical Review Letters, 2012, 109, 256601.	2.9	19
56	Thermodynamic properties of a two-dimensional electron gas with attractive interactions. Physical Review B, 1992, 45, 8197-8200.	1.1	18
57	Slave-boson mean-field theory for the negative-UHubbard model. Physical Review B, 1992, 45, 377-382.	1.1	18
58	Bilayer graphene under pressure: Electron-hole symmetry breaking, valley Hall effect, and Landau levels. Physical Review B, 2016, 93, .	1.1	18
59	Heavy Dirac fermions in a graphene/topological insulator hetero-junction. 2D Materials, 2016, 3, 034006.	2.0	18
60	Low-Energy Phases of Bi Monolayer Predicted by Structure Search in Two Dimensions. Journal of Physical Chemistry Letters, 2019, 10, 7324-7332.	2.1	18
61	Screening of charged impurities as a possible mechanism for conductance change in graphene gas sensing. Physical Review B, 2014, 90, .	1.1	16
62	Bond Polarizability Model for Sum Frequency Generation at the Al₂O₃(0001)â€“H₂O Interface. Journal of Physical Chemistry A, 2017, 121, 3045-3055.	1.1	16
63	Electronic structure ofBaPb1â^'xBixO3. Physical Review B, 1989, 39, 9701-9703.	1.1	15
64	Effect of the local charge disproportionation on the electronic structure ofBaPb1â^'xBixO3. Physical Review B, 1989, 40, 6955-6962.	1.1	15
65	One-particle excitations in strong-coupling superconductors: A new realization of thet-Jmodel. Physical Review B, 1990, 42, 10241-10244.	1.1	14
66	Transport coefficients and thermoelectric figure of merit ofnâ€Hg1â^'xCdxTe. Journal of Applied Physics, 1994, 76, 2249-2254.	1.1	14
67	Theory of genus reduction in alkali-induced graphitization of nanoporous carbon. Physical Review B, 2007, 76, .	1.1	14
68	Anion Photoelectron Spectroscopy and Density Functional Investigation of Diniobiumâ^'Carbon Clusters. ACS Nano, 2007, 1, 319-326.	7.3	14
69	Dispersion of edge states and quantum confinement of electrons in graphene channels drawn on graphene fluoride. Physical Review B, 2011, 83, .	1.1	14
70	First-Principles Investigation of Laves Phases in Mg-Al-Ca System. Materials Science Forum, 2005, 488-489, 169-176.	0.3	13
71	Diffusion and transport coefficients in synthetic opals. Physical Review B, 2000, 62, 2780-2785.	1.1	12
72	Photoemission study of the skutterudite compounds CoSb3and RhSb3. Journal of the Physical Society of Japan, 2002, 71, 2271-2275.	0.7	12

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73	Analysis of periodic SchrÃ¶dinger operators: Regularity and approximation of eigenfunctions. Journal of Mathematical Physics, 2008, 49, 083501.	0.5	12
74	Adsorption of Zn²⁺ on the (110) Surface of TiO₂ (Rutile): A Density Functional Molecular Dynamics Study. Journal of Physical Chemistry C, 2011, 115, 9608-9614.	1.5	12
75	Structural, electronic, optical and vibrational properties of nanoscale carbons and nanowires: a colloquial review. Journal of Physics Condensed Matter, 2010, 22, 334201.	0.7	10
76	Novel substrates for Helium adsorption: Graphane and Grapheneâ€"Fluoride. Journal of Physics: Conference Series, 2012, 400, 012010.	0.3	10
77	First-principles studies of lattice dynamics and thermal properties of Mg₂Si_{1â^'x}Sn_x. Journal of Materials Research, 2015, 30, 2578-2584.	1.2	10
78	Critical behavior of Young's modulus for two-dimensional randomly holed metallized Mylar. Physical Review B, 1987, 36, 3960-3962.	1.1	9
79	Fully retarded van der Waals interaction between dielectric nanoclusters. Journal of Chemical Physics, 2006, 125, 174303.	1.2	7
80	The Electrical Conductivity of Strontium-Barium Niobate. Journal of Electronic Materials, 2013, 42, 1375-1376.	1.0	7
81	How do insertions affect green fluorescent protein?. Chemical Physics Letters, 2006, 419, 48-54.	1.2	6
82	Broad photoelectron spectrum and lowered electron affinity due to hydrogen in ZnOH: A joint experimental and theoretical study. Journal of Chemical Physics, 2012, 136, 214314.	1.2	6
83	Hydrogen movement in cubicMg2NiH4. Physical Review B, 2002, 65, .	1.1	5
84	Coverage dependence study of the adsorption of Pd on MoS2(). Surface Science, 2002, 506, 161-171.	0.8	5
85	Ground state of the attractive-UHubbard model. Physical Review Letters, 1992, 68, 896-896.	2.9	4
86	Multiple isomers in the photoelectron spectra of small mono-niobium carbide clusters. Journal of Chemical Physics, 2011, 134, 184310.	1.2	4
87	Thermoelectric figure of merit ofnâ€Hg1â^'xCdxSe. Journal of Applied Physics, 1995, 77, 1561-1563.	1.1	3
88	Ortho-para conversion of H2 in crystalline silicon. , 2010, , .		2
89	Landau level phases in bilayer graphene under pressure at charge neutrality. Physical Review B, 2020, 101, .	1.1	1
90	Inversion domain boundaries in wurtzite GaN. Physical Review B, 2021, 103, .	1.1	1

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91	New Phases in Mg-Al-Ca System. , 2016, , 427-432.		1
92	Charge distribution in GaAsâ€Ga1â^'xAlxAs heterostructures under an external magnetic field. Applied Physics Letters, 1988, 53, 282-284.	1.5	0
93	Protein simulations in confined environments. , 2004, , .		0
94	Peter Clay Eklund: a scientific biography. Journal of Physics Condensed Matter, 2010, 22, 330301.	0.7	0
95	Calculation of the orthoâ€“para conversion of hydrogen in apâ€“type silicon lattice using a dwell time approach. Journal of Physics: Conference Series, 2012, 397, 012064.	0.3	0