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	Inversion domain boundaries in wurtzite GaN. Physical Review B, 2021, 103, .	1.1	1
2	Landau level phases in bilayer graphene under pressure at charge neutrality. Physical Review B, 2020, 101, .	1.1	1
3	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
4	Bending energy of 2D materials: graphene, MoS₂ and imogolite. RSC Advances, 2018, 8, 4577-4583.	1.7	26
5	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
6	Bilayer graphene under pressure: Electron-hole symmetry breaking, valley Hall effect, and Landau levels. Physical Review B, 2016, 93, .	1.1	18
7	Effect of Ions on H-Bond Structure and Dynamics at the Quartz(101)â€“Water Interface. Langmuir, 2016, 32, 11353-11365.	1.6	41
8	Heavy Dirac fermions in a graphene/topological insulator hetero-junction. 2D Materials, 2016, 3, 034006.	2.0	18
9	New Phases in Mg-Al-Ca System. , 2016, , 427-432.		1
10	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
11	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
12	Screening of charged impurities as a possible mechanism for conductance change in graphene gas sensing. Physical Review B, 2014, 90, .	1.1	16
13	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
14	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
15	The Electrical Conductivity of Strontium-Barium Niobate. Journal of Electronic Materials, 2013, 42, 1375-1376.	1.0	7
16	Analysis and optimization of carbon nanotubes and graphene sensors based on adsorption-desorption kinetics. Applied Physics Letters, 2013, 103, .	1.5	21
17	Development of a ReaxFF Reactive Force Field for Titanium Dioxide/Water Systems. Langmuir, 2013, 29, 7838-7846.	1.6	96
18	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

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19	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
20	Comment on â€œStructure and dynamics of liquid water on rutile TiO2(110)â€• Physical Review B, 2012, 85, .	1.1	46
21	Impurity State and Variable Range Hopping Conduction in Graphene. Physical Review Letters, 2012, 109, 256601.	2.9	19
22	A New Hypothesis for the Dissolution Mechanism of Silicates. Journal of Physical Chemistry C, 2012, 116, 17479-17491.	1.5	52
23	Novel substrates for Helium adsorption: Graphane and Grapheneâ€”Fluoride. Journal of Physics: Conference Series, 2012, 400, 012010.	0.3	10
24	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
25	Magnetic structure of hydrogen-induced defects on graphene. Physical Review B, 2012, 85, .	1.1	46
26	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
27	Gate-Voltage Control of Oxygen Diffusion on Graphene. Physical Review Letters, 2011, 106, 146802.	2.9	99
28	Dispersion of edge states and quantum confinement of electrons in graphene channels drawn on graphene fluoride. Physical Review B, 2011, 83, .	1.1	14
29	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
30	Faster proton transfer dynamics of water on SnO2 compared to TiO2. Journal of Chemical Physics, 2011, 134, 044706.	1.2	34
31	Electrical control of the chemical bonding of fluorine on graphene. Physical Review B, 2011, 83, .	1.1	76
32	Oxygen migration on the graphene surface. 2. Thermochemistry of basal-plane diffusion (hopping). Carbon, 2011, 49, 4226-4238.	5.4	78
33	Multiple isomers in the photoelectron spectra of small mono-niobium carbide clusters. Journal of Chemical Physics, 2011, 134, 184310.	1.2	4
34	Peter Clay Eklund: a scientific biography. Journal of Physics Condensed Matter, 2010, 22, 330301.	0.7	0
35	Ortho-para conversion of H2 in crystalline silicon. , 2010, , .		2
36	Reversible fluorination of graphene: Evidence of a two-dimensional wide bandgap semiconductor. Physical Review B, 2010, 81, .	1.1	365

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37	Photoluminescence from nanocrystalline graphite monofluoride. Applied Physics Letters, 2010, 97, .	1.5	31
38	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
39	Hydrogen Bonds and Vibrations of Water on (110) Rutile. Journal of Physical Chemistry C, 2009, 113, 13732-13740.	1.5	74
40	n-Type Behavior of Graphene Supported on Si/SiO₂ Substrates. ACS Nano, 2008, 2, 2037-2044.	7.3	241
41	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
42	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
43	Analysis of periodic SchrÃ¶dinger operators: Regularity and approximation of eigenfunctions. Journal of Mathematical Physics, 2008, 49, 083501.	0.5	12
44	Theory of genus reduction in alkali-induced graphitization of nanoporous carbon. Physical Review B, 2007, 76, .	1.1	14
45	Anion Photoelectron Spectroscopy and Density Functional Investigation of Diniobiumâ^'Carbon Clusters. ACS Nano, 2007, 1, 319-326.	7.3	14
46	Van der Waals Dispersion Forces between Dielectric Nanoclusters. Langmuir, 2007, 23, 1735-1740.	1.6	73
47	Graphane: A two-dimensional hydrocarbon. Physical Review B, 2007, 75, .	1.1	1,744
48	van der Waals forces between nanoclusters: Importance of many-body effects. Journal of Chemical Physics, 2006, 124, 074504.	1.2	57
49	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
50	Anion Photoelectron Spectroscopy and Density Functional Investigation of Vanadium Carbide Clusters. Journal of Physical Chemistry A, 2006, 110, 12814-12821.	1.1	22
51	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
52	Thermodynamics modeling of the Mgâ€“Sr and Caâ€“Mgâ€“Sr systems. Journal of Alloys and Compounds, 2006, 421, 172-178.	2.8	41
53	Contribution of first-principles energetics to the Caâ€“Mg thermodynamic modeling. Journal of Alloys and Compounds, 2006, 420, 98-106.	2.8	36
54	Linear optical properties of solids within the full-potential linearized augmented planewave method. Computer Physics Communications, 2006, 175, 1-14.	3.0	1,215

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55	How do insertions affect green fluorescent protein?. Chemical Physics Letters, 2006, 419, 48-54.	1.2	6
56	Fully retarded van der Waals interaction between dielectric nanoclusters. Journal of Chemical Physics, 2006, 125, 174303.	1.2	7
57	Electronic structure calculations of physisorption and chemisorption on oxide glass surfaces. Physical Review B, 2005, 72, .	1.1	44
58	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
59	First-Principles Investigation of Laves Phases in Mg-Al-Ca System. Materials Science Forum, 2005, 488-489, 169-176.	0.3	13
60	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
61	Static polarizabilities of dielectric nanoclusters. Physical Review A, 2005, 72, .	1.0	46
62	An integrated framework for multi-scale materials simulation and design. Journal of Computer-Aided Materials Design, 2004, 11, 183-199.	0.7	46
63	First-principles study of binary bcc alloys using special quasirandom structures. Physical Review B, 2004, 69, .	1.1	266
64	Scanning Tunneling Microscopy Chemical Signature of Point Defects on theMoS2(0001)Surface. Physical Review Letters, 2004, 92, 026802.	2.9	105
65	Improved thermoelectric devices using bismuth alloys. Applied Physics Letters, 2004, 85, 588-590.	1.5	32
66	Protein simulations in confined environments. , 2004, , .		0
67	Stress-induced defects inSb2Te3. Physical Review B, 2003, 68, .	1.1	77
68	Thermoelectric properties ofSb2Te3under pressure and uniaxial stress. Physical Review B, 2003, 68, .	1.1	175
69	Transport coefficients from first-principles calculations. Physical Review B, 2003, 68, .	1.1	663
70	Hydrogen movement in cubicMg2NiH4. Physical Review B, 2002, 65, .	1.1	5
71	Electronic structure of the pyrochlore metalsCd2Os2O7andCd2Re2O7. Physical Review B, 2002, 65, .	1.1	81
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	Coverage dependence study of the adsorption of Pd on MoS2(). Surface Science, 2002, 506, 161-171.	0.8	5
74	Metal-insulator transition in the double perovskites. Physical Review B, 2001, 64, .	1.1	28
75	Diffusion and transport coefficients in synthetic opals. Physical Review B, 2000, 62, 2780-2785.	1.1	12
76	Calculation of the electronic and structural properties of cubicMg2NiH4. Physical Review B, 1999, 59, 11746-11754.	1.1	63
77	Adsorption of Pd onMoS2(1000):Ab initioelectronic-structure calculations. Physical Review B, 1999, 60, 8343-8347.	1.1	32
78	Electronic structure ofCoSb3:A narrow-band-gap semiconductor. Physical Review B, 1998, 58, 15620-15623.	1.1	179
79	Multilayer thermionic refrigerator and generator. Journal of Applied Physics, 1998, 83, 4683-4689.	1.1	148
80	The best thermoelectric.. Proceedings of the National Academy of Sciences of the United States of America, 1996, 93, 7436-7439.	3.3	1,385
81	Thermoelectric figure of merit ofnâ€Hg1â^'xCdxSe. Journal of Applied Physics, 1995, 77, 1561-1563.	1.1	3
82	Transport coefficients and thermoelectric figure of merit ofnâ€Hg1â^'xCdxTe. Journal of Applied Physics, 1994, 76, 2249-2254.	1.1	14
83	Optimum band gap of a thermoelectric material. Physical Review B, 1994, 49, 4565-4570.	1.1	221
84	Thermoelectric figure of merit of superlattices. Applied Physics Letters, 1994, 65, 2690-2692.	1.5	167
85	Resistivity and superconductivity from anharmonic phonons. Physical Review B, 1993, 47, 8050-8055.	1.1	33
86	Thermodynamic properties of a two-dimensional electron gas with attractive interactions. Physical Review B, 1992, 45, 8197-8200.	1.1	18
87	Slave-boson mean-field theory for the negative-UHubbard model. Physical Review B, 1992, 45, 377-382.	1.1	18
88	Ground state of the attractive-UHubbard model. Physical Review Letters, 1992, 68, 896-896.	2.9	4
89	Collective excitations in superconductors: From Bardeen-Cooper-Schrieffer theory to Bose condensation. Physical Review B, 1992, 45, 9860-9864.	1.1	26
90	Intrinsic bistability in resonant-tunneling structures. Physical Review B, 1990, 42, 7292-7295.	1.1	31

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91	One-particle excitations in strong-coupling superconductors: A new realization of thet-Jmodel. Physical Review B, 1990, 42, 10241-10244.	1.1	14
92	Electronic structure ofBaPb1â^'xBixO3. Physical Review B, 1989, 39, 9701-9703.	1.1	15
93	Effect of the local charge disproportionation on the electronic structure ofBaPb1â^'xBixO3. Physical Review B, 1989, 40, 6955-6962.	1.1	15
94	Charge distribution in GaAsâ€Ga1â^'xAlxAs heterostructures under an external magnetic field. Applied Physics Letters, 1988, 53, 282-284.	1.5	0
95	Critical behavior of Young's modulus for two-dimensional randomly holed metallized Mylar. Physical Review B, 1987, 36, 3960-3962.	1.1	9