Apostolos G Marinopoulos

List of Publications by Year
in descending order

48 papers	1,490 citations	361413 20 h-index	315739 38 g-index
48 all docs	48 docs citations	48 times ranked	1450 citing authors

#	Article	IF	Citations
1	Linear Plasmon Dispersion in Single-Wall Carbon Nanotubes and the Collective Excitation Spectrum of Graphene. Physical Review Letters, 2008, 100, 196803.	7.8	211
2	Ab initiostudy of the optical absorption and wave-vector-dependent dielectric response of graphite. Physical Review B, 2004, 69, .	3.2	175
3	Optical and Loss Spectra of Carbon Nanotubes: Depolarization Effects and Intertube Interactions. Physical Review Letters, 2003, 91, 046402.	7.8	174
4	Anisotropy and Interplane Interactions in the Dielectric Response of Graphite. Physical Review Letters, 2002, 89, 076402.	7.8	119
5	Optical absorption and electron energy loss spectra of carbon and boron nitride nanotubes: a first-principles approach. Applied Physics A: Materials Science and Processing, 2004, 78, 1157-1167.	2.3	105
6	TDDFT from molecules to solids: The role of long-range interactions. International Journal of Quantum Chemistry, 2005, 102, 684-701.	2.0	65
7	Quantitative Atomic-Scale Analysis of Interface Structures: Transmission Electron Microscopy and Local Density Functional Theory. Physical Review Letters, 2001, 86, 5066-5069.	7.8	63
8	Microscopic structure and bonding at the rhombohedral twin interface in Î±-Al2O3. Acta Materialia, 2000, 48, 4375-4386.	7.9	60
9	Interfacial structures and energetics of basal twins inÎ±â^'Al2O3:First-principles density-functional and empirical calculations. Physical Review B, 2001, 63, .	3.2	42
10	Significance of non-central forces in atomistic studies of grain boundaries in bcc transition metals. Philosophical Magazine A: Physics of Condensed Matter, Structure, Defects and Mechanical Properties, 1995, 72, 1311-1330.	0.6	38
11	Hydrogen impurity in yttria:Ab initioand<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mi>Î¼</mml:mi></mml:math>SR perspectives. Physical Review B, 2012, 85, .	3.2	32
12	Substitutional cation impurities in Î±-Al2O3: ab-initio case study of segregation to the rhombohedral twin boundary. Acta Materialia, 2001, 49, 2951-2959.	7.9	31
13	Hydrogen shuttling near Hf-defect complexes in Siâ•SiO2â•HfO2 structures. Applied Physics Letters, 2007, 91, .	3.3	30
14	Density-functional and shell-model calculations of the energetics of basal-plane stacking faults in sapphire. Philosophical Magazine Letters, 2001, 81, 329-338.	1.2	28
15	Performance, reliability, radiation effects, and aging issues in microelectronics â€“ From atomic-scale physics to engineering-level modeling. Solid-State Electronics, 2010, 54, 841-848.	1.4	24
16	Hydrogen impurity in paratellurite<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:mi>Î±</mml:mi></mml:mrow></mml:math>-TeO<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow /><mml:mrow><mml:mn>2</mml:mn></mml:mrow></mml:msub></mml:mrow></mml:math>: Muon-spin rotation andab initiostudies. Physical Review B, 2011, 84, .	3.2	24
17	Isolated hydrogen configurations in zirconia as seen by muon spin spectroscopy andab initiocalculations. Physical Review B, 2016, 94, .	3.2	24
18	Anomalous Angular Dependence of the Dynamic Structure Factor near Bragg Reflections: Graphite. Physical Review Letters, 2008, 101, 266406.	7.8	23

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19	Incorporation and migration of hydrogen in yttria-stabilized cubic zirconia: Insights from semilocal and hybrid-functional calculations. Physical Review B, 2012, 86, .	3.2	23
20	Electronic structure of interstitial hydrogen in lutetium oxide from<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mtext>DFT</mml:mtext><mml:mo>+</mml:mo><mml:mi>U</mml:mi></m and comparison study with<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:mi>Î¼</mml:mi><mml:mi>SR</mml:mi></mml:mrow></mml Physical Review B, 2016, 94, .	3.2	21
21	Titanium in silicon: Lattice positions and electronic properties. Applied Physics Letters, 2014, 104, 152105.	3.3	20
22	Ab initiostudy of the dielectric response of crystalline ropes of metallic single-walled carbon nanotubes: Tube-diameter and helicity effects. Physical Review B, 2008, 78, .	3.2	16
23	DFT+<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mi>U</mml:mi></mml:math>study of electrical levels and migration barriers of early<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:mn>3</mml:mn><mml:mi>d</mml:mi></mml:mrow></mml:r <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:mn>4</mml:mn><mml:mi>d</mml:mi></mml:mrow></mml:r metals in silicon. Physical Review B, 2015, 92.	3.2	16
24	Impurity segregation and ordering in<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:mtext>Si</mml:mtext><mml:mo>/</mml:mo><mml:msub><mml:mrow><mml:mtext>SiO</mml:mtext></mml:mt Physical Review B, 2008, 77, .	3.2	13
25	Defect levels and hyperfine constants of hydrogen in beryllium oxide from hybrid-functional calculations and muonium spectroscopy. Philosophical Magazine, 2017, 97, 2108-2128.	1.6	13
26	Local and Effective Elastic Properties of Grain Boundaries in Silicon. Physica Status Solidi A, 1998, 166, 453-473.	1.7	12
27	Local-field and excitonic effects in the optical response of<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:mi>Î±</mml:mi></mml:mrow></mml:math>-alumina. Physical Review B, 2011, 83, .	3.2	12
28	Recombination via transition metals in solar silicon: The significance of hydrogenâ€“metal reactions and lattice sites of metal atoms. Physica Status Solidi (A) Applications and Materials Science, 2017, 214, 1700304.	1.8	11
29	Protons in cubic yttria-stabilized zirconia: Binding sites and migration pathways. Solid State Ionics, 2018, 315, 116-125.	2.7	9
30	First-principles study of the formation energies and positron lifetimes of vacancies in the Yttrium-Aluminum Garnet Y3Al5O12. European Physical Journal B, 2019, 92, 1.	1.5	9
31	Electronic structure and migration of interstitial hydrogen in the rutile phase of TiO2. Journal of Physics Condensed Matter, 2018, 30, 425503.	1.8	8
32	First-principles study of hydrogen configurations at the core of a high-angle grain boundary in cubic yttria-stabilized zirconia. Journal of Physics Condensed Matter, 2014, 26, 025502.	1.8	7
33	Muon-Spin-Rotation study of yttria-stabilized zirconia (ZrO2:Y): Evidence for muon and electron separate traps. Journal of Physics: Conference Series, 2014, 551, 012050.	0.4	6
34	First principles study of segregation to the Î£5(310) grain boundary of cubic zirconia. Journal of Physics Condensed Matter, 2011, 23, 085005.	1.8	5
35	Hydrogen states in mixed-cation CuIn(1-x)GaxSe2 chalcopyrite alloys: a combined study by first-principles density-functional calculations and muon-spin spectroscopy. Philosophical Magazine, 0, , 1-23.	1.6	5
36	Positron lifetimes of bare and hydrogenated zirconium vacancies in cubic yttria-stabilized zirconia: an ab initio study. Journal of Physics Condensed Matter, 2019, 31, 315503.	1.8	4

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37	xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mi>Î±</mml:mi><mml:mo>â^'</mml:mo><mml:mrow><mml:msub><mml:mathvariant="normal">O</mml:mi><mml:mn>3</mml:mn></mml:msub></mml:mrow></mml:math> puzzle: Joint <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:mi>Î¼</mml:mi><mml:mi>SR</mml:mi></mml:mrow></mml:math> and density functional theory study. Physical Review B, 2021, 103, .	3.2	3
38	Optical absorption in small BN and C nanotubes. AIP Conference Proceedings, 2003, , .	0.4	2
39	Performance, reliability, radiation effects, and aging issues in microelectronics - from atomic-scale physics to engineering-level modeling. , 2009, , .		2
40	Performance, reliability, radiation effects, and aging issues in microelectronics — from atomic-scale physics to engineering-level modeling. , 2009, , .		2
41	Performance, Reliability, Radiation Effects, and Aging Issues in Microelectronics - From Atomic-Scale Physics to Engineering-Level Modeling. ECS Transactions, 2009, 19, 319-337.	0.5	1
42	Electrical Levels and Diffusion Barriers of Early 3d and 4d Transition Metals in Silicon. Solid State Phenomena, 0, 242, 264-270.	0.3	1
43	Binding and energetics of oxygen at the CuInSe₂ chalcopyrite and the CuInSe₂/CdS interface. Physica Scripta, 0, , .	2.5	1
44	Microscopic Analysis of Twin Grain Boundaries in Alumina. Microscopy and Microanalysis, 2001, 7, 312-313.	0.4	0
45	Seeing inside materials by aberration-corrected electron microscopy. International Journal of Nanotechnology, 2011, 8, 935.	0.2	0
46	Zr vacancies and their complexes with hydrogen in monoclinic zirconia: formation energies and positron lifetimes. Physica Scripta, 2020, 95, 035801.	2.5	0
47	Microscopic Characterization of Devices by Scanning Transmission Electron Microscopy: From Single Atom Imaging to Macroscopic Properties. , 2009, , .		0
48	Interaction of hydrogen impurities with intrinsic point defects at the CuInSe$$_2$$/CdS interface of chalcopyrite-based solar cells. European Physical Journal B, 2022, 95, 1.	1.5	0