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	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
2	Sapphire <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mi>Î±</mml:mi><mml:mo>â^'</mml:mo><mml:mrow><mml:msub><mml:mi 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 and density functional theory study. Physical Review B, 2021, 103, .	3.2	3
3	Zr vacancies and their complexes with hydrogen in monoclinic zirconia: formation energies and positron lifetimes. Physica Scripta, 2020, 95, 035801.	2.5	0
4	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
5	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
6	Protons in cubic yttria-stabilized zirconia: Binding sites and migration pathways. Solid State Ionics, 2018, 315, 116-125.	2.7	9
7	Electronic structure and migration of interstitial hydrogen in the rutile phase of TiO2. Journal of Physics Condensed Matter, 2018, 30, 425503.	1.8	8
8	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
9	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
10	Isolated hydrogen configurations in zirconia as seen by muon spin spectroscopy andab initiocalculations. Physical Review B, 2016, 94, .	3.2	24
11	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> 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></m DFT+<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mi>U</mml:mi></mml:math>study of	3.2	21
12	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
13	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
14	Titanium in silicon: Lattice positions and electronic properties. Applied Physics Letters, 2014, 104, 152105.	3.3	20
15	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
16	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
17	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
18	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

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19	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
20	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
21	Seeing inside materials by aberration-corrected electron microscopy. International Journal of Nanotechnology, 2011, 8, 935.	0.2	0
22	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
23	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
24	Performance, reliability, radiation effects, and aging issues in microelectronics - from atomic-scale physics to engineering-level modeling. , 2009, , .		2
25	Performance, reliability, radiation effects, and aging issues in microelectronics — from atomic-scale physics to engineering-level modeling. , 2009, , .		2
26	Microscopic Characterization of Devices by Scanning Transmission Electron Microscopy: From Single Atom Imaging to Macroscopic Properties. , 2009, , .		0
27	Linear Plasmon Dispersion in Single-Wall Carbon Nanotubes and the Collective Excitation Spectrum of Graphene. Physical Review Letters, 2008, 100, 196803.	7.8	211
28	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
29	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:mrow><mml:mrow><mml:mn>2</mml:mn></mml:mrow></mml:msub></mml:mrow></mml:math>: Physical Review B, 2008, 77, .	3.2	0
30	Anomalous Angular Dependence of the Dynamic Structure Factor near Bragg Reflections: Graphite. Physical Review Letters, 2008, 101, 266406.	7.8	23
31	Hydrogen shuttling near Hf-defect complexes in Siâˆ•SiO2âˆ•HfO2 structures. Applied Physics Letters, 2007, 91, .	3.3	30
32	TDDFT from molecules to solids: The role of long-range interactions. International Journal of Quantum Chemistry, 2005, 102, 684-701.	2.0	65
33	Ab initiostudy of the optical absorption and wave-vector-dependent dielectric response of graphite. Physical Review B, 2004, 69, .	3.2	175
34	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
35	Optical and Loss Spectra of Carbon Nanotubes: Depolarization Effects and Intertube Interactions. Physical Review Letters, 2003, 91, 046402.	7.8	174
36	Optical absorption in small BN and C nanotubes. AIP Conference Proceedings, 2003, , .	0.4	2

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37	Anisotropy and Interplane Interactions in the Dielectric Response of Graphite. Physical Review Letters, 2002, 89, 076402.	7.8	119
38	Microscopic Analysis of Twin Grain Boundaries in Alumina. Microscopy and Microanalysis, 2001, 7, 312-313.	0.4	0
39	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
40	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
41	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
42	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
43	Microscopic structure and bonding at the rhombohedral twin interface in Î±-Al2O3. Acta Materialia, 2000, 48, 4375-4386.	7.9	60
44	Local and Effective Elastic Properties of Grain Boundaries in Silicon. Physica Status Solidi A, 1998, 166, 453-473.	1.7	12
45	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
46	Electrical Levels and Diffusion Barriers of Early 3d and 4d Transition Metals in Silicon. Solid State Phenomena, 0, 242, 264-270.	0.3	1
47	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
48	Binding and energetics of oxygen at the CuInSe₂ chalcopyrite and the CuInSe₂/CdS interface. Physica Scripta, 0, , .	2.5	1