Roberto H Miwa

List of Publications by Year
in descending order

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119	2,841	185998 28	197535 49
papers	citations	h-index	g-index

120	120	120	3806
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Electronic and Transport Properties of Boron-Doped Graphene Nanoribbons. Physical Review Letters, 2007, 98, 196803.	2.9	540
2	Electronic, structural, and transport properties of Ni-doped graphene nanoribbons. Physical Review B, 2009, 79, .	1.1	143
3	Ïƒ- and Ï€-Defects at Graphene Nanoribbon Edges: Building Spin Filters. Nano Letters, 2008, 8, 2293-2298.	4.5	101
4	Metal Chalcogenides Janus Monolayers for Efficient Hydrogen Generation by Photocatalytic Water Splitting. ACS Applied Nano Materials, 2019, 2, 890-897.	2.4	93
5	Directional dependence of the electronic and transport properties of 2D borophene and borophane. Physical Chemistry Chemical Physics, 2016, 18, 25491-25496.	1.3	92
6	Hydrogen adsorption on boron doped graphene: anab initiostudy. Nanotechnology, 2008, 19, 155708.	1.3	86
7	Two-dimensional van der Waals p-n junction of InSe/phosphorene. Physical Review B, 2017, 95, .	1.1	68
8	Ferromagnetic coupling in a Co-doped graphenelike ZnO sheet. Physical Review B, 2010, 81, .	1.1	62
9	Ab initiostudy of native defects in SiC nanotubes. Physical Review B, 2006, 74, .	1.1	59
10	Electronic and structural properties of germanium self-interstitials. Physical Review B, 2004, 70, .	1.1	55
11	First-Principles Calculations of Carbon Nanotubes Adsorbed on Si(001). Physical Review Letters, 2003, 91, 166802.	2.9	54
12	Topological insulator Bi<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mrow /><mml:mn>2</mml:mn></mml:msub></mml:math>Se<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mrow /><mml:mn>3</mml:mn></mml:msub></mml:math>(111) surface doped with transition metals: Anab initioinvestigation. Physical Review B, 2013, 88, .	1.1	52
13	Spin texture and magnetic anisotropy of Co impurities in Bi<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mrow /><mml:mn>2</mml:mn></mml:msub></mml:math>Se<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mrow /><mml:mn>3</mml:mn></mml:msub></mml:math>topological insulators. Physical Review B, 2011, 84, .	1.1	47
14	Doping of graphene adsorbed on the a-SiO2 surface. Applied Physics Letters, 2011, 99, 163108.	1.5	46
15	B and N doping in graphene ruled by grain boundary defects. Physical Review B, 2012, 85, .	1.1	46
16	Layer-dependent band alignment of few layers of blue phosphorus and their van der Waals heterostructures with graphene. Physical Review B, 2018, 97, .	1.1	45
17	Large disparity between optical and fundamental band gaps in layered <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:msub><mml:mi>In</mml:mi><mml:mn>2</mml:mn></mml:msub></mml:mrow></mml:math>Se<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:msub><mml:mi>In</mml:mi><mml:mn>2</mml:mn></mml:msub></mml:mrow></mml:math>. Physical Review B, 2018, 98, .	1.1	41
18	Hydrogen interaction with native defects in<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:mi>SiC</mml:mi></mml:mrow></mml:math>nanotubes. Physical Review B, 2007, 76, .	1.1	39

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19	Topological flat band, Dirac fermions and quantum spin Hall phase in 2D Archimedean lattices. Physical Chemistry Chemical Physics, 2019, 21, 22344-22350.	1.3	39
20	Lithium incorporation at the MoS₂/graphene interface: anab initioinvestigation. Journal of Physics Condensed Matter, 2013, 25, 445301.	0.7	36
21	Stability and electronic confinement of free-standingInPnanowires:Ab initiocalculations. Physical Review B, 2005, 72, .	1.1	35
22	Substrate-dependent electronic properties of an armchair carbon nanotube adsorbed on Hâˆ•Si(001). Applied Physics Letters, 2005, 86, 213111.	1.5	34
23	Bi covered Si(111) surface revisited. Journal of Physics Condensed Matter, 2003, 15, 2441-2447.	0.7	33
24	Boron and nitrogen impurities in SiC nanowires. Physical Review B, 2009, 79, .	1.1	32
25	Oxidation of free-standing and supported borophene. 2D Materials, 2017, 4, 025025.	2.0	31
26	Quenching of local magnetic moment in oxygen adsorbed graphene nanoribbons. Journal of Chemical Physics, 2008, 128, 201101.	1.2	29
27	Hydrogenated grain boundaries in graphene. Applied Physics Letters, 2011, 98, .	1.5	29
28	Adsorption and diffusion of gold adatoms on graphene nanoribbons: Anab initiostudy. Physical Review B, 2010, 82, .	1.1	28
29	Topological phases in triangular lattices of Ru adsorbed on graphene:Ab initiocalculations. Physical Review B, 2014, 89, .	1.1	25
30	The equilibrium geometry and electronic structure of Bi nanolines on clean and hydrogenated Si(001) surfaces. Nanotechnology, 2005, 16, 2427-2435.	1.3	24
31	Ab initiostudy of TCNQ-doped carbon nanotubes. Physical Review B, 2006, 73, .	1.1	23
32	Stability and electronic properties of native defects and substitutional impurities in GaN nanotubes. Journal of Applied Physics, 2008, 104, 033712.	1.1	23
33	Organic molecules deposited on graphene: A computational investigation of self-assembly and electronic structure. Journal of Chemical Physics, 2015, 142, 044301.	1.2	23
34	Mechanical and electronic properties of SiC nanowires: An ab initio study. Journal of Applied Physics, 2017, 121, .	1.1	22
35	Topological states ruled by stacking faults in Bi2Se3 and Bi2Te3. Journal of Applied Physics, 2013, 113, 023705.	1.1	21
36	Electronic stripes and transport properties in borophene heterostructures. Nanoscale, 2019, 11, 17894-17903.	2.8	21

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37	Energetic stability, equilibrium geometry, and the electronic properties ofCaâˆ•Si(111)surfaces. Physical Review B, 2005, 72, .	1.1	19
38	Self-organized Bi lines on the Si(001) surface:â€ƒA theoretical study. Physical Review B, 2002, 66, .	1.1	18
39	Doping effects of C, Si and Ge in wurtzite [0001] GaN, AlN, and InN nanowires. Journal of Applied Physics, 2011, 110, .	1.1	18
40	The electronic origin of contrast reversal in bias-dependent STM images of nanolines. Surface Science, 2005, 576, 116-122.	0.8	17
41	Adsorption of metal-phthalocyanine molecules onto the Si(111) surface passivated by<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mi>Î´</mml:mi></mml:math>doping:Ab initiocalculations. Physical Review B, 2016, 93, .	1.1	17
42	A new class of large band gap quantum spin hall insulators: 2D fluorinated group-IV binary compounds. Scientific Reports, 2016, 6, 26123.	1.6	17
43	Orbital Pseudospin-Momentum Locking in Two-Dimensional Chiral Borophene. Nano Letters, 2019, 19, 6564-6568.	4.5	17
44	Confinement and fermion doubling problem in Dirac-like Hamiltonians. Physical Review B, 2017, 96, .	1.1	16
45	Probing the local interface properties at a grapheneâ€“MoSe₂ in-plane lateral heterostructure: an ab initio study. Physical Chemistry Chemical Physics, 2018, 20, 17952-17960.	1.3	16
46	Fe adatoms along Bi nanolines on Hâˆ•Si(001). Applied Physics Letters, 2006, 89, 093105.	1.5	15
47	Mn dimers on graphene nanoribbons: An ab initio study. Journal of Applied Physics, 2011, 109, 053715.	1.1	15
48	Tuning the topological states in metal-organic bilayers. Physical Review B, 2017, 96, .	1.1	15
49	Double flat bands in kagome twisted bilayers. Physical Review B, 2019, 100, .	1.1	15
50	Layertronic control of topological states in multilayer metal-organic frameworks. Journal of Chemical Physics, 2019, 150, 234701.	1.2	15
51	The geometry of Bi nanolines on Si(001). Applied Surface Science, 2005, 244, 157-160.	3.1	14
52	Quantum anomalous Hall effect in metal-bis(dithiolene), magnetic properties, doping and interfacing graphene. Physical Chemistry Chemical Physics, 2018, 20, 22652-22659.	1.3	14
53	Anab initiostudy of energetic stability and electronic confinement for different structural phases of ZnO nanowires. Nanotechnology, 2009, 20, 215202.	1.3	13
54	Unveiling the dopant segregation effect at hematite interfaces. Applied Physics Letters, 2021, 118, .	1.5	13

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55	Jacutingaite-family: A class of topological materials. Physical Review B, 2020, 102, .	1.1	13
56	Structural, electronic, and magnetic properties of pristine and oxygen-adsorbed graphene nanoribbons. Applied Surface Science, 2010, 256, 5776-5782.	3.1	12
57	Graphene on amorphous HfO2surface: Anab initioinvestigation. Physical Review B, 2013, 87, .	1.1	12
58	Self-assembly of NiTPP on Cu(111): a transition from disordered 1D wires to 2D chiral domains. Physical Chemistry Chemical Physics, 2015, 17, 18344-18352.	1.3	12
59	Electronic and optical properties of hydrogenated group-IV multilayer materials. Physical Chemistry Chemical Physics, 2018, 20, 8112-8118.	1.3	12
60	The electronic properties of Si(001)â€“Bi(2 Ã— n). Journal of Physics Condensed Matter, 2005, 17, 571-580.	0.7	11
61	Templating an organic array with Si(111)-7Ã—7. Chemical Communications, 2011, 47, 8031.	2.2	11
62	Valley Hall effect in silicene and hydrogenated silicene ruled by grain boundaries: Anab initioinvestigation. Physical Review B, 2015, 91, .	1.1	11
63	MoS2 on an amorphous HfO2 surface: An ab initio investigation. Journal of Applied Physics, 2015, 117, 194303.	1.1	11
64	Templating an organic layer with the Si(111)-<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:mn>7</mml:mn><mml:mo>Ã—</mml:mo><mml:mn>7</mml:mn></mml:mrow></mml:math>surface reconstruction using steric constraints. Physical Review B, 2011, 84, .	1.1	10
65	Topological phase transitions of (BixSb1â^'x)2Se3 alloys by density functional theory. Journal of Physics Condensed Matter, 2015, 27, 255501.	0.7	10
66	InP and InAs nanowires hetero- and homojunctions: energetic stability and electronic properties. Nanotechnology, 2010, 21, 285204.	1.3	9
67	Switchable magnetic moment in cobalt-doped graphene bilayer on Cu(111): Anab initiostudy. Physical Review B, 2016, 93, .	1.1	9
68	Tunable magnetism and spin-polarized electronic transport in graphene mediated by molecular functionalization of extended defects. Physical Review B, 2018, 97, .	1.1	9
69	Graphene on the oxidized SiC surface and the impact of the metal intercalation. Carbon, 2019, 145, 603-613.	5.4	9
70	Oxygen intercalated graphene on SiC(0001): Multiphase SiOx layer formation and its influence on graphene electronic properties. Carbon, 2020, 167, 746-759.	5.4	9
71	Theoretical investigations of Sb-induced(3Ã—8)and(1Ã—3)reconstructions on theGaAs(111)Bsurface. Physical Review B, 2001, 63, .	1.1	8
72	Carbon inSixGe1â^'x:Anab initioinvestigation. Physical Review B, 2004, 69, .	1.1	8

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73	Electronic steps and band offset ofSiâˆ'Getwo-dimensional superlattices onBiâˆ•Si(111). Physical Review B, 2005, 72, .	1.1	8
74	In nanolines and nanoclusters on self-assembled Bi-lines. Surface Science, 2006, 600, 4048-4051.	0.8	8
75	Energetic stability, equilibrium geometry, and electronic properties of Bi-inducedSi(001)â˜'(2Ã—n)surfaces. Physical Review B, 2006, 74, .	1.1	8
76	Ab initiostudy of thiophene chemisorption on<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:mtext>Si</mml:mtext><mml:mrow><mml:mo>(</mml:mo><mml:mrow><mml:mn>111</mml:mn> Physical Review B, 2009, 80, .	1.1	8
77	Machine Learning of Microscopic Ingredients for Graphene Oxide/Cellulose Interaction. Langmuir, 2022, 38, 1124-1130.	1.6	8
78	Carbon nanotube adsorbed on hydrogenated Si(001) surfaces. Applied Surface Science, 2005, 244, 124-128.	3.1	7
79	Piezomagnetic behavior of Co-doped ZnO nanoribbons. Physical Review B, 2011, 84, .	1.1	7
80	Graphene and graphene nanoribbons on InAs(110) and Au/InAs(110) surfaces: Anab initiostudy. Physical Review B, 2011, 84, .	1.1	7
81	[PIn](n)antisite clustering in InP. Physical Review B, 1999, 60, 16475-16478.	1.1	6
82	Bismuth nanolines on Si(001) and their influence on mesoscopic surface structure. Materials Science and Technology, 2004, 20, 951-954.	0.8	6
83	EL2-like defects in InP nanowires: Anab initiototal energy investigation. Physical Review B, 2007, 75, .	1.1	6
84	Theoretical investigation of Mn adsorbates aside self-organised Bi nanolines on hydrogenated Si(001) surface. Surface Science, 2008, 602, 2789-2795.	0.8	6
85	Iron silicide wires patterned by Bi nanolines on the H/Si(001) surface: Spin density functional calculations. Physical Review B, 2008, 78, .	1.1	6
86	Simulations of X-ray absorption spectroscopy and energetic conformation of N-heterocyclic carbenes on Au(111). Physical Chemistry Chemical Physics, 2020, 22, 21504-21511.	1.3	6
87	Disassembly of TEMPO-Oxidized Cellulose Fibers: Intersheet and Interchain Interactions in the Isolation of Nanofibers and Unitary Chains. Journal of Physical Chemistry B, 2021, 125, 3717-3724.	1.2	6
88	Structural models and core-level shifts of the oxidation of the Si(001) surface. Physical Review B, 2004, 70, .	1.1	5
89	Anomalous gap dependence of stretched Teflonâˆ•poly(p-phenylene vinylene) films. Applied Physics Letters, 2005, 86, 141907.	1.5	5
90	The role of a precursor state in thiophene chemisorption on Si(111)-7Ã—7. Physica Status Solidi C: Current Topics in Solid State Physics, 2010, 7, 240-243.	0.8	5

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91	Carrier-mediated magnetism in transition metal doped Bi2Se3 topological insulator. Journal of Physics Condensed Matter, 2013, 25, 445003.	0.7	5
92	Electronic confinement in graphene ruled by N doped extended defects. Nanotechnology, 2014, 25, 245706.	1.3	5
93	Periodic arrays of intercalated atoms in twisted bilayer graphene: Anab initioinvestigation. Physical Review B, 2015, 92, .	1.1	5
94	Nanolines of transition metals ruled by grain boundaries in graphene: An ab initio study. Materials Chemistry and Physics, 2017, 194, 118-127.	2.0	5
95	Retention of contaminants Cd and Hg adsorbed and intercalated in aluminosilicate clays: A first principles study. Journal of Chemical Physics, 2017, 147, 174704.	1.2	5
96	Theoretical investigation of extended defects and their interactions with vacancies inSixGe1âˆ’x. Physical Review B, 2003, 67, .	1.1	4
97	Structural Transition in Oxidized Ca2N Electrenes: CaO/CaN 2D Heterostructures. Journal of Physical Chemistry C, 2020, 124, 14706-14712.	1.5	4
98	Engineering Metal-sp_{xy} Dirac Bands on the Oxidized SiC Surface. Nano Letters, 2020, 20, 3956-3962.	4.5	4
99	Magnetic switch and electronic properties in chromium-intercalated two-dimensional <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mi>GeP</mml:mi><mml:mn>3</mml:mn></mml:msub></mml:math> Physical Review Materials, 2021, 5, .	0.9	4
100	Reply to Comment on â€˜Bi nanolines on Si(001): registry with the substrateâ€™. Nanotechnology, 2006, 17, 1803-1805.	1.3	3
101	Benzene adsorption and the encapsulation processes in SiC nanotubes. Journal of Applied Physics, 2012, 112, 023702.	1.1	3
102	Ab initioinvestigation of the electronic properties of graphene on InAs(111)A. Journal of Physics Condensed Matter, 2012, 24, 485004.	0.7	3
103	Surface and near surface defects inÎ´-doped Si(1â€‰1â€‰1). Journal of Physics Condensed Matter, 2015, 27, 125001.	0.7	3
104	Tuning the p-type Schottky barrier in 2D metal/semiconductor interface:boron-sheet on MoSe2, and WSe2. Journal of Physics Condensed Matter, 2017, 29, 405002.	0.7	3
105	An ab initio investigation of Bi₂Se₃ topological insulator deposited on amorphous SiO₂. Journal of Physics Condensed Matter, 2017, 29, 045302.	0.7	3
106	The role played by the molecular geometry on the electronic transport through nanometric organic films. Physical Chemistry Chemical Physics, 2019, 21, 24584-24591.	1.3	3
107	Tuning band offsets at the AlAs/GaAs interface by group-IV intralayer deposition. Physical Review B, 1999, 59, 12499-12504.	1.1	2
108	Gold adatoms and clusters on PPV: Anab initioinvestigation. Journal of Chemical Physics, 2010, 133, 204703.	1.2	2

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109	Pyridine intercalated Bi2Se3heterostructures: controlling the topologically protected states. Nanotechnology, 2016, 27, 035704.	1.3	2
110	Electronic Properties of the Weyl Semimetals Co₂MnX (X=Si, Ge, Sn). Physica Status Solidi - Rapid Research Letters, 2022, 16, .	1.2	2
111	Tuning Low-Spin to High-Spin Mn Pairs in 2-D ZnO by Injecting Holes. IEEE Nanotechnology Magazine, 2012, 11, 71-76.	1.1	1
112	Electronic and structural properties of nitrogen adsorbed Nb(100) surfaces: An ab initio study. Journal of Applied Physics, 2013, 114, 063705.	1.1	1
113	H₂O incorporation in the phosphorene/a-SiO₂interface: a first-principles study. Journal of Physics Condensed Matter, 2017, 29, 075002.	0.7	1
114	Investigating the preservation of Ï€â€“conjugation in covalently functionalized carbon nanotubes through first principles simulations. Journal of Chemical Physics, 2019, 150, 204701.	1.2	1
115	Oxidation of two-dimensional electrides: Structural transition and the formation of half-metallic channels protected by oxide layers. Physical Review B, 2022, 105, .	1.1	1
116	Inhibiting molecular array formation on Si(111)-<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:mn>7</mml:mn><mml:mo>Ã—</mml:mo><mml:mn>7</mml:mn></mml:mrow></mml:math>using site-selective Ge/Si exchange. Physical Review B, 2012, 85, .	1.1	0
117	Using steric constraints to template an organic array on Si(111)â€7â€‰Ã—â€‰7. Physica Status Solidi (A) Applications and Materials Science, 2012, 209, 647-652.	0.8	0
118	Nanodots of transition metal dichalcogenides embedded in MoS2 and MoSe2: first-principles calculations. Physical Chemistry Chemical Physics, 2017, 19, 26240-26247.	1.3	0
119	Tuning the electronic transport properties in few-layers GeP<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline" id="d1e899" altimg="si9.svg"><mml:msub><mml:mrow /><mml:mrow><mml:mn>3</mml:mn></mml:mrow></mml:msub></mml:math> intercalated by Cr-atoms. Physica E: Low-Dimensional Systems and Nanostructures, 2022, 141, 115242.	1.3	0