

Sohrab Ismail-Beigi

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108
papers

6,278
citations

42
h-index

78
g-index

118
ext. papers

6,913
ext. citations

6.6
avg, IF

6.18
L-index

#	Paper	IF	Citations
108	Excitonic effects and optical spectra of single-walled carbon nanotubes. <i>Physical Review Letters</i> , 2004 , 92, 077402	7.4	805
107	Novel precursors for boron nanotubes: the competition of two-center and three-center bonding in boron sheets. <i>Physical Review Letters</i> , 2007 , 99, 115501	7.4	629
106	Theory and ab initio calculation of radiative lifetime of excitons in semiconducting carbon nanotubes. <i>Physical Review Letters</i> , 2005 , 95, 247402	7.4	248
105	Truncation of periodic image interactions for confined systems. <i>Physical Review B</i> , 2006 , 73,	3.3	207
104	Crystalline oxides on silicon. <i>Advanced Materials</i> , 2010 , 22, 2919-38	24	180
103	Ab initio study of screw dislocations in Mo and ta: A new picture of plasticity in bcc transition metals. <i>Physical Review Letters</i> , 2000 , 84, 1499-502	7.4	172
102	Large-area single-crystal sheets of borophene on Cu(111) surfaces. <i>Nature Nanotechnology</i> , 2019 , 14, 44-49	28.7	171
101	Diameter and chirality dependence of exciton properties in carbon nanotubes. <i>Physical Review B</i> , 2006 , 74,	3.3	168
100	Locality of the Density Matrix in Metals, Semiconductors, and Insulators. <i>Physical Review Letters</i> , 1999 , 82, 2127-2130	7.4	164
99	First-principles study of boron sheets and nanotubes. <i>Physical Review B</i> , 2010 , 82,	3.3	144
98	Quasiparticle energies, excitonic effects and optical absorption spectra of small-diameter single-walled carbon nanotubes. <i>Applied Physics A: Materials Science and Processing</i> , 2004 , 78, 1129-1136 ^{2.6}		126
97	Self-doping in boron sheets from first principles: A route to structural design of metal boride nanostructures. <i>Physical Review B</i> , 2009 , 80,	3.3	124
96	Effect of semicore orbitals on the electronic band gaps of Si, Ge, and GaAs within the GW approximation. <i>Physical Review B</i> , 2004 , 69,	3.3	114
95	Orbital engineering in symmetry-breaking polar heterostructures. <i>Physical Review Letters</i> , 2015 , 114, 026801	7.4	109
94	Photoisomerization of azobenzene from first-principles constrained density-functional calculations. <i>Journal of Chemical Physics</i> , 2005 , 122, 094311	3.9	108
93	Electronic and magnetic properties of SrTiO(3)/LaAlO(3) interfaces from first principles. <i>Advanced Materials</i> , 2010 , 22, 2881-99	24	95
92	Ferroelectrics: A pathway to switchable surface chemistry and catalysis. <i>Surface Science</i> , 2016 , 650, 302-316	3.6	94

91	Quasiparticle band structure of ZnS and ZnSe. <i>Physical Review B</i> , 2002 , 66,	3.3	92
90	Ferroelectric-Based Catalysis: Switchable Surface Chemistry. <i>ACS Catalysis</i> , 2015 , 5, 4537-4545	13.1	90
89	Excited-state forces within a first-principles Green's function formalism. <i>Physical Review Letters</i> , 2003 , 90, 076401	7.4	84
88	Tuning the structure of nickelates to achieve two-dimensional electron conduction. <i>Advanced Materials</i> , 2014 , 26, 1935-40	24	81
87	Self-trapped excitons in silicon dioxide: mechanism and properties. <i>Physical Review Letters</i> , 2005 , 95, 156401	7.4	79
86	Ferroelectric oxide surface chemistry: water splitting via pyroelectricity. <i>Journal of Materials Chemistry A</i> , 2016 , 4, 5235-5246	13	78
85	New algebraic formulation of density functional calculation. <i>Computer Physics Communications</i> , 2000 , 128, 1-45	4.2	78
84	Ferroelectric surface chemistry: First-principles study of the PbTiO ₃ surface. <i>Physical Review B</i> , 2013 , 88,	3.3	77
83	Chemistry of ferroelectric surfaces. <i>Advanced Materials</i> , 2010 , 22, 2969-73	24	76
82	Interface-induced polarization and inhibition of ferroelectricity in epitaxial SrTiO ₃ /Si. <i>Physical Review Letters</i> , 2010 , 105, 217601	7.4	62
81	Alkaline earth stannates: The next silicon?. <i>APL Materials</i> , 2015 , 3, 062510	5.7	61
80	LaTiO ₃ /KTaO ₃ interfaces: A new two-dimensional electron gas system. <i>APL Materials</i> , 2015 , 3, 036104	5.7	60
79	Modifying the electronic orbitals of nickelate heterostructures via structural distortions. <i>Physical Review Letters</i> , 2013 , 110, 186402	7.4	59
78	Role of strontium in oxide epitaxy on silicon (001). <i>Physical Review Letters</i> , 2008 , 101, 105503	7.4	59
77	Reversible modulation of orbital occupations via an interface-induced polar state in metallic manganites. <i>Nano Letters</i> , 2014 , 14, 4965-70	11.5	58
76	Comparison of drive currents in metal-oxide-semiconductor field-effect transistors made of Si, Ge, GaAs, InGaAs, and InAs channels. <i>Applied Physics Letters</i> , 2010 , 96, 122105	3.4	55
75	Polarization-driven catalysis via ferroelectric oxide surfaces. <i>Physical Chemistry Chemical Physics</i> , 2016 , 18, 19676-95	3.6	55
74	Fundamental asymmetry in interfacial electronic reconstruction between insulating oxides: An ab initio study. <i>Physical Review B</i> , 2009 , 79,	3.3	51

73	Coupling of nonlocal potentials to electromagnetic fields. <i>Physical Review Letters</i> , 2001 , 87, 087402	7.4	51
72	Edge-driven transition in the surface structure of nanoscale silicon. <i>Physical Review B</i> , 1998 , 57, 11923-11926	3.3	47
71	Controlled doping of carbon nanotubes with metallocenes for application in hybrid carbon nanotube/Si solar cells. <i>Nano Letters</i> , 2014 , 14, 3388-94	11.5	45
70	Selection rules for one- and two-photon absorption by excitons in carbon nanotubes. <i>Physical Review B</i> , 2006 , 73,	3.3	43
69	Elasticity of nanometer-sized objects. <i>Physical Review B</i> , 2002 , 65,	3.3	43
68	Ferroelectric control of magnetization in $\text{La}_{1-x}\text{Sr}_x\text{MnO}_3$ manganites: A first-principles study. <i>Physical Review B</i> , 2012 , 86,	3.3	42
67	Atomic structure of the epitaxial BaO/Si(001) interface. <i>Physical Review Letters</i> , 2009 , 102, 116101	7.4	42
66	Ab initio and finite-temperature molecular dynamics studies of lattice resistance in tantalum. <i>Physical Review B</i> , 2003 , 68,	3.3	42
65	Electronic excitations in single-walled GaN nanotubes from first principles: Dark excitons and unconventional diameter dependences. <i>Physical Review B</i> , 2008 , 77,	3.3	38
64	Conduction at a Ferroelectric Interface. <i>Physical Review Applied</i> , 2014 , 2,	4.3	37
63	Role of double TiO_2 layers at the interface of $\text{FeSe}/\text{SrTiO}_3$ superconductors. <i>Physical Review B</i> , 2016 , 93,	3.3	35
62	Nature of Lone-Pair-Surface Bonds and Their Scaling Relations. <i>Inorganic Chemistry</i> , 2018 , 57, 7222-7238	5.1	35
61	Directed self-assembly of hybrid oxide/polymer core/shell nanowires with transport optimized morphology for photovoltaics. <i>Advanced Materials</i> , 2012 , 24, 82-7	24	35
60	Importance of anisotropic Coulomb interaction in LaMnO_3 . <i>Physical Review B</i> , 2015 , 92,	3.3	35
59	First-principles study of electronic reconstructions of $\text{LaAlO}_3/\text{SrTiO}_3$ heterointerfaces and their variants. <i>Physical Review B</i> , 2010 , 82,	3.3	35
58	Causes of ferroelectricity in HfO -based thin films: an ab initio perspective. <i>Physical Chemistry Chemical Physics</i> , 2019 , 21, 12150-12162	3.6	34
57	How Correlated is the $\text{FeSe}/\text{SrTiO}_3$ System?. <i>Physical Review Letters</i> , 2017 , 119, 067004	7.4	34
56	Effect of Surface Termination on the Electronic Properties of LaNiO_3 Films. <i>Physical Review Applied</i> , 2014 , 2,	4.3	34

55	Picoscale materials engineering. <i>Nature Reviews Materials</i> , 2017 , 2,	73.3	33
54	Interface structure and film polarization in epitaxial SrTiO ₃ /Si(001). <i>Physical Review B</i> , 2012 , 85,	3.3	31
53	Phase diagram of Sr on Si(001): A first-principles study. <i>Physical Review B</i> , 2009 , 80,	3.3	31
52	Dynamic evanescent phonon coupling across the La(1-x)Sr(x)MnO ₃ /SrTiO ₃ interface. <i>Physical Review Letters</i> , 2011 , 107, 105501	7.4	31
51	Accurate tight-binding Hamiltonian matrices from ab initio calculations: Minimal basis sets. <i>Physical Review B</i> , 2016 , 93,	3.3	29
50	Excitons in carbon nanotubes: Diameter and chirality trends. <i>Physica Status Solidi (B): Basic Research</i> , 2007 , 244, 4016-4020	1.3	29
49	Directing the Structure of Two-Dimensional Silica and Silicates. <i>Journal of Physical Chemistry C</i> , 2016 , 120, 26770-26781	3.8	28
48	Electric field tuned crossover from classical to weakly localized quantum transport in electron doped SrTiO ₃ . <i>Physical Review B</i> , 2010 , 81,	3.3	28
47	Research Update: Orbital polarization in LaNiO ₃ -based heterostructures. <i>APL Materials</i> , 2015 , 3, 062303	5.7	27
46	First-principles study of oxygen-deficient LaNiO ₃ structures. <i>Physical Review B</i> , 2015 , 92,	3.3	26
45	Intrinsic interfacial phenomena in manganite heterostructures. <i>Journal of Physics Condensed Matter</i> , 2015 , 27, 123001	1.8	22
44	Thermodynamic stability and growth kinetics of epitaxial SrTiO ₃ on silicon. <i>Physical Review B</i> , 2011 , 83,	3.3	21
43	Correlation energy functional within the GW-RPA: Exact forms, approximate forms, and challenges. <i>Physical Review B</i> , 2010 , 81,	3.3	20
42	Mechanism for strong binding of CdSe quantum dots to multiwall carbon nanotubes for solar energy harvesting. <i>Nanoscale</i> , 2013 , 5, 6893-900	7.7	18
41	Quasiparticle and Excitonic Effects in the Optical Response of Nanotubes and Nanoribbons. <i>Topics in Applied Physics</i> , 2007 , 195-227	0.5	17
40	Excited-state forces within time-dependent density-functional theory: A frequency-domain approach. <i>Physical Review A</i> , 2007 , 76,	2.6	17
39	Paramagnetic Structure of the Soliton of the 30° Partial Dislocation in Silicon. <i>Physical Review Letters</i> , 1998 , 80, 3984-3987	7.4	17
38	Single Atomic Layer Ferroelectric on Silicon. <i>Nano Letters</i> , 2018 , 18, 241-246	11.5	16

37	Deciphering the atomic structure of a complex Sr/Ge (100) phase via scanning tunneling microscopy and first-principles calculations. <i>Physical Review B</i> , 2012 , 85,	3-3	12
36	Free energy of the concerted-exchange mechanism for self-diffusion in silicon. <i>Physical Review B</i> , 1996 , 53, 1310-1314	3-3	12
35	Growth and interfacial properties of epitaxial oxides on semiconductors: ab initio insights. <i>Journal of Materials Science</i> , 2012 , 47, 7417-7438	4-3	11
34	Ab initio study of the BaTiO ₃ /Ge interface. <i>Physical Review B</i> , 2017 , 96,	3-3	10
33	Generalized slave-particle method for extended Hubbard models. <i>Physical Review B</i> , 2015 , 92,	3-3	10
32	Strong Orbital Polarization in a Cobaltate-Titanate Oxide Heterostructure. <i>Physical Review Letters</i> , 2019 , 123, 117201	7-4	9
31	Theory of Ferroelectric ZrO ₂ Monolayers on Si. <i>Journal of Physical Chemistry C</i> , 2019 , 123, 14350-14361	3-8	9
30	Complex-time shredded propagator method for large-scale GW calculations. <i>Physical Review B</i> , 2020 , 101,	3-3	9
29	Experimental verification of orbital engineering at the atomic scale: Charge transfer and symmetry breaking in nickelate heterostructures. <i>Physical Review B</i> , 2017 , 95,	3-3	9
28	Imaging the buried MgO/Ag interface: Formation mechanism of the STM contrast. <i>Physical Review B</i> , 2014 , 90,	3-3	9
27	Phase transition of Sr on Si (001): First principles prediction and experiment. <i>Surface Science</i> , 2010 , 604, 857-861	1-8	9
26	Control of hidden ground-state order in NdNiO ₃ superlattices. <i>Physical Review Materials</i> , 2017 , 1,	3-2	9
25	Controlling Mobility in Perovskite Oxides by Ferroelectric Modulation of Atomic-Scale Interface Structure. <i>Nano Letters</i> , 2018 , 18, 573-578	11-5	8
24	Designing and controlling the properties of transition metal oxide quantum materials. <i>Nature Materials</i> , 2021 , 20, 1462-1468	2-7	8
23	Surface Piezoelectricity of (0001) Sapphire. <i>Physical Review Applied</i> , 2019 , 11,	4-3	7
22	Diffraction studies of submonolayer Sr structures on the Si (001) surface. <i>Journal of Vacuum Science & Technology B</i> , 2009 , 27, 2015		7
21	Revealing surface-state transport in ultrathin topological crystalline insulator SnTe films. <i>APL Materials</i> , 2019 , 7, 051106	5-7	6
20	Formation and atomic structure of ordered Sr-induced nanostrips on Ge(100). <i>Physical Review B</i> , 2014 , 89,	3-3	6

19	Two-dimensional electron gas oxide remote doping of Si(001). <i>Physical Review Materials</i> , 2018 , 2,	3.2	6
18	Length Scale and Dimensionality of Defects in Epitaxial SnTe Topological Crystalline Insulator Films. <i>Advanced Materials Interfaces</i> , 2017 , 4, 1601011	4.6	5
17	Tuning two-dimensional phase formation through epitaxial strain and growth conditions: silica and silicate on NiPd(111) alloy substrates. <i>Nanoscale</i> , 2019 , 11, 21340-21353	7.7	5
16	Scalable GW software for quasiparticle properties using OpenAtom. <i>Computer Physics Communications</i> , 2019 , 244, 427-441	4.2	4
15	Justifying quasiparticle self-consistent schemes via gradient optimization in Baym-Kadanoff theory. <i>Journal of Physics Condensed Matter</i> , 2017 , 29, 385501	1.8	4
14	First principles calculation of optical and electronic properties with inclusion of exciton effects. <i>Physica Status Solidi C: Current Topics in Solid State Physics</i> , 2006 , 3, 3365-3372		4
13	Structure of a Two-Dimensional Silicate Layer Formed by Reaction with an Alloy Substrate. <i>Chemistry of Materials</i> , 2019 , 31, 851-861	9.6	4
12	Magnetism of (LaCoO ₃) _n +(LaTiO ₃) _n superlattices (n=1,2). <i>Physical Review B</i> , 2020 , 101,	3.3	3
11	Suppression of the spectral weight of topological surface states on the nanoscale via local symmetry breaking. <i>Physical Review Materials</i> , 2018 , 2,	3.2	3
10	Growth of ultrathin Ru oxide films on perovskite and corundum substrates. <i>Surface Science</i> , 2019 , 688, 51-62	1.8	2
9	Ferroelectric ZrO ₂ Monolayers as Buffer Layers between SrTiO ₃ and Si. <i>Journal of Physical Chemistry C</i> , 2019 , 123, 15053-15061	3.8	2
8	Charge transfer and negative curvature energy in magnesium boride nanotubes. <i>Physical Review B</i> , 2016 , 94,	3.3	2
7	Symmetry breaking in occupation number based slave-particle methods. <i>Physical Review B</i> , 2017 , 96,	3.3	2
6	New physics of the 30° partial dislocation in silicon revealed through ab initio calculation. <i>Journal of Physics Condensed Matter</i> , 2000 , 12, 10029-10037	1.8	2
5	Micrometre-scale single-crystalline borophene on a square-lattice Cu(100) surface. <i>Nature Chemistry</i> , 2022 ,	17.6	2
4	Origin of the orbital polarization of Co ²⁺ in La ₂ CoTiO ₆ and (LaCoO ₃) ₁ +(LaTiO ₃) ₁ : A DFT+U and DFMT study. <i>Physical Review B</i> , 2021 , 103,	3.3	2
3	Boson Subsidiary Solver (BoSS) v1.1. <i>Computer Physics Communications</i> , 2021 , 265, 107991	4.2	1
2	Experimental and theoretical investigation of the formation of two-dimensional Fe silicate on Pd(111). <i>Journal of Vacuum Science and Technology A: Vacuum, Surfaces and Films</i> , 2021 , 39, 062201	2.9	0

- 1 Identifying crystal structures and chemical reactions at the interface of stanene on Bi₂Te₃. *Journal of Applied Physics*, **2020**, 128, 165301 2.5