Sohrab Ismail-Beigi

List of Publications by Year
in descending order

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114 papers	7,541 citations	57758 44 h-index	53230 85 g-index
118 all docs	118 docs citations	118 times ranked	8363 citing authors

#	Article	IF	Citations
1	Micrometre-scale single-crystalline borophene on a square-lattice Cu(100) surface. Nature Chemistry, 2022, 14, 377-383.	13.6	28
2	Epitaxial binding and strain effects of monolayer stanene on the Al2O3(0001) surface. Physical Review Materials, 2022, 6, .	2.4	0
3	Toward Complete Exfoliation of the Chemisorbed Two-Dimensional Iron Silicates on Ru(0001) via Hydrogenation. Journal of Physical Chemistry C, 2022, 126, 11769-11778.	3.1	2
4	Origin of the orbital polarization of <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msup><mml:mrow><mml:mi>Co</mml:mi></mml:mrow><mml:mrow><m in <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:msub><mml:mi>La</mml:mi><mml:mn>2</mml:mn></mml:r		

#	Article	IF	Citations
19	Revealing surface-state transport in ultrathin topological crystalline insulator SnTe films. APL Materials, 2019, 7, .	5.1	9
20	Causes of ferroelectricity in HfO₂-based thin films: an ab initio perspective. Physical Chemistry Chemical Physics, 2019, 21, 12150-12162.	2.8	56
21	Tuning two-dimensional phase formation through epitaxial strain and growth conditions: silica and silicate on Ni_xPd_{1â^'x}(111) alloy substrates. Nanoscale, 2019, 11, 21340-21353.	5.6	11
22	Degree of locality of elasto-optic response in solids. Physical Review B, 2019, 100, .	3.2	2
23	Structure of a Two-Dimensional Silicate Layer Formed by Reaction with an Alloy Substrate. Chemistry of Materials, 2019, 31, 851-861.	6.7	11
24	Large-area single-crystal sheets of borophene on Cu(111) surfaces. Nature Nanotechnology, 2019, 14, 44-49.	31.5	285
25	Controlling Mobility in Perovskite Oxides by Ferroelectric Modulation of Atomic-Scale Interface Structure. Nano Letters, 2018, 18, 573-578.	9.1	17
26	Single Atomic Layer Ferroelectric on Silicon. Nano Letters, 2018, 18, 241-246.	9.1	26
27	Nature of Lone-Pairâ€“Surface Bonds and Their Scaling Relations. Inorganic Chemistry, 2018, 57, 7222-7238.	4.0	43
28	Suppression of the spectral weight of topological surface states on the nanoscale via local symmetry breaking. Physical Review Materials, 2018, 2, .	2.4	3
29	Two-dimensional electron gas oxide remote doping of Si(001). Physical Review Materials, 2018, 2, .	2.4	7
30	Length Scale and Dimensionality of Defects in Epitaxial SnTe Topological Crystalline Insulator Films. Advanced Materials Interfaces, 2017, 4, 1601011.	3.7	6
31	Crystalline Insulators: Length Scale and Dimensionality of Defects in Epitaxial SnTe Topological Crystalline Insulator Films (Adv. Mater. Interfaces 2/2017). Advanced Materials Interfaces, 2017, 4, .	3.7	1
32	Picoscale materials engineering. Nature Reviews Materials, 2017, 2, .	48.7	42
33	Ab initio study of the <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:msub><mml:mi>BaTiO</mml:mi><mml:mn>3</mml:mn></mml:msub></mml:mrow></mml:math> interface. Physical Review B, 2017, 96, .	3.2	11
34	How Correlated is the <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:mi>FeSe</mml:mi><mml:mo>/</mml:mo><mml:msub><mml:mrow><mml:mi>SrTiO</mml:mi></mml:mrow></mml:msub></mml:mrow></mml:math> System?. Physical Review Letters, 2017, 119, 067004.	7.8	44
35	Symmetry breaking in occupation number based slave-particle methods. Physical Review B, 2017, 96, .	3.2	8
36	Justifying quasiparticle self-consistent schemes via gradient optimization in Baymâ€“Kadanoff theory. Journal of Physics Condensed Matter, 2017, 29, 385501.	1.8	15

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37	Experimental verification of orbital engineering at the atomic scale: Charge transfer and symmetry breaking in nickelate heterostructures. Physical Review B, 2017, 95, .	3.2	12
38	Control of hidden ground-state order in <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:mi>NdNi</mml:mi><mml:msub><mml:mi mathvariant="normal">O</mml:mi><mml:mn>3</mml:mn></mml:msub></mml:mrow></mml:math> superlattices. Physical Review Materials, 2017, 1, .	2.4	12
39	Polarization-driven catalysis via ferroelectric oxide surfaces. Physical Chemistry Chemical Physics, 2016, 18, 19676-19695.	2.8	65
40	Accurate tight-binding Hamiltonian matrices fromab initiocalculations: Minimal basis sets. Physical Review B, 2016, 93, .	3.2	43
41	Role of double <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:mi>Ti</mml:mi><mml:msub><mml:mi mathvariant="normal">O</mml:mi><mml:mn>2</mml:mn></mml:msub></mml:mrow></mml:math>layers at the interface of FeSe/<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:mi>SrTi</mml:mi><mml:msub><mml:mi mathvariant="normal">O</mml:mi><mml:mn>3</mml:mn></mml:msub></mml:mrow></mml:math>superconductors.	3.2	40
42	Charge transfer and negative curvature energy in magnesium boride nanotubes. Physical Review B, 2016, 94, .	3.2	2
43	Directing the Structure of Two-Dimensional Silica and Silicates. Journal of Physical Chemistry C, 2016, 120, 26770-26781.	3.1	36
44	Ferroelectric oxide surface chemistry: water splitting via pyroelectricity. Journal of Materials Chemistry A, 2016, 4, 5235-5246.	10.3	99
45	Ferroelectrics: A pathway to switchable surface chemistry and catalysis. Surface Science, 2016, 650, 302-316.	1.9	114
46	First-principles study of oxygen-deficient<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mi>LaNiO</mml:mi><mml:mn>3</mml:mn></mml:msub></mml:math> Physical Review B, 2015, 92, .	3.2	42
47	Generalized slave-particle method for extended Hubbard models. Physical Review B, 2015, 92, .	3.2	15
48	Importance of anisotropic Coulomb interaction in<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mi>LaMnO</mml:mi><mml:mn>3</mml:mn></mml:msub></mml:math> Physical Review B, 2015, 92, .	3.2	47
49	Research Update: Orbital polarization in LaNiO₃-based heterostructures. APL Materials, 2015, 3, 062303.	5.1	34
50	Orbital Engineering in Symmetry-Breaking Polar Heterostructures. Physical Review Letters, 2015, 114, 026801.	7.8	135
51	Intrinsic interfacial phenomena in manganite heterostructures. Journal of Physics Condensed Matter, 2015, 27, 123001.	1.8	25
52	Ferroelectric-Based Catalysis: Switchable Surface Chemistry. ACS Catalysis, 2015, 5, 4537-4545.	11.2	122
53	LaTiO3/KTaO3 interfaces: A new two-dimensional electron gas system. APL Materials, 2015, 3, .	5.1	94
54	Alkaline earth stannates: The next silicon?. APL Materials, 2015, 3, 062510.	5.1	71

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55	Imaging the buried MgO/Ag interface: Formation mechanism of the STM contrast. Physical Review B, 2014, 90, .	3.2	12
56	Effect of Surface Termination on the Electronic Properties of<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow><mml:mi>LaNiO</mml:mi></mml:mrow><mml:mrow><mml:mn>3</mml:mn><mml:mo>â^’</mml:mo><mml:mi>x</mml:mi></mml:mrow></mml:msub></mml:mrow></mml:math>. Physical Review Applied, 2014, 2, .	3.8	45
57	Formation and atomic structure of ordered Sr-induced nanostrips on Ge(100). Physical Review B, 2014, 89, .	3.2	6
58	Conduction at a Ferroelectric Interface. Physical Review Applied, 2014, 2, .	3.8	41
59	Tuning the Structure of Nickelates to Achieve Twoâ€Dimensional Electron Conduction. Advanced Materials, 2014, 26, 1935-1940.	21.0	99
60	Controlled Doping of Carbon Nanotubes with Metallocenes for Application in Hybrid Carbon Nanotube/Si Solar Cells. Nano Letters, 2014, 14, 3388-3394.	9.1	53
61	Reversible Modulation of Orbital Occupations via an Interface-Induced Polar State in Metallic Manganites. Nano Letters, 2014, 14, 4965-4970.	9.1	61
62	Modifying the Electronic Orbitals of Nickelate Heterostructures via Structural Distortions. Physical Review Letters, 2013, 110, 186402.	7.8	69
63	Mechanism for strong binding of CdSe quantum dots to multiwall carbon nanotubes for solar energy harvesting. Nanoscale, 2013, 5, 6893.	5.6	18
64	Ferroelectric surface chemistry: First-principles study of the PbTiO<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>surface. Physical Review B, 2013, 88, .	3.2	87
65	Deciphering the atomic structure of a complex Sr/Ge (100) phase via scanning tunneling microscopy and first-principles calculations. Physical Review B, 2012, 85, .	3.2	12
66	Growth and interfacial properties of epitaxial oxides on semiconductors: ab initio insights. Journal of Materials Science, 2012, 47, 7417-7438.	3.7	12
67	Ferroelectric control of magnetization in La<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mrow /><mml:mrow><mml:mn>1</mml:mn><mml:mo>â^’</mml:mo><mml:mi>x</mml:mi></mml:mrow></mml:msub></mml:math>Sr<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mrow /><mml:mi>x</mml:mi></mml:msub></mml:math>MnO<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mrow	3.2	42
68	Interface structure and film polarization in epitaxial SrTiO<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>/Si(001). Physical Review B, 2012, 85, .	3.2	37
69	Directed Selfâ€Assembly of Hybrid Oxide/Polymer Core/Shell Nanowires with Transport Optimized Morphology for Photovoltaics. Advanced Materials, 2012, 24, 82-87.	21.0	37
70	Thermodynamic stability and growth kinetics of epitaxial SrTiO<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow /><mml:mrow><mml:mn>3</mml:mn></mml:mrow></mml:msub></mml:mrow></mml:math>on silicon. Physical Review B, 2011, 83, .	3.2	22
71	Dynamic Evanescent Phonon Coupling Across the<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mi>La</mml:mi><mml:mrow><mml:mn>1</mml:mn><mml:mo>â^’</mml:mo><mml:mi>x</mml:mi></mml:mrow></mml:msub></mml:math>/<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mi>Sr</mml:mi><mml:mi>x</mml:mi></mml:msub></mml:math>/<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mi>Ti</mml:mi><mml:mi>O</mml:mi></mml:msub></mml:math>Interface. Physical Review Letters, 2011, 107, 105501.	7.8	38
72	Chemistry of Ferroelectric Surfaces. Advanced Materials, 2010, 22, 2969-2973.	21.0	86

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73	Electronic and Magnetic Properties of SrTiO₃/LaAlO₃ Interfaces from First Principles. Advanced Materials, 2010, 22, 2881-2899.	21.0	107
74	Crystalline Oxides on Silicon. Advanced Materials, 2010, 22, 2919-2938.	21.0	203
75	Phase transition of Sr on Si (001): First principles prediction and experiment. Surface Science, 2010, 604, 857-861.	1.9	9
76	Correlation energy functional within the<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:mi>G</mml:mi><mml:mi>W</mml:mi></mml:mrow></mml:math>-RPA: Exact forms, approximate forms, and challenges. Physical Review B, 2010, 81, .	3.2	22
77	Interface-Induced Polarization and Inhibition of Ferroelectricity in Epitaxial<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mi>SrTiO</mml:mi><mml:mn>3</mml:mn></mml:msub><mml:mo>/</mml:mo><mml:mi>Si</mml:mi> Physical Review Letters, 2010, 105, 217601.	7.8	65
78	Electric field tuned crossover from classical to weakly localized quantum transport in electron doped<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow><mml:mtext>SrTiO</mml:mtext></mml:mrow><mml:mn>3</mml:mn></mml:msub></mml:mrow> Physical Review B, 2010, 81, .	3.2	31
79	First-principles study of electronic reconstructions ofLaAlO3/SrTiO3heterointerfaces and their variants. Physical Review B, 2010, 82, .	3.2	44
80	First-principles study of boron sheets and nanotubes. Physical Review B, 2010, 82, .	3.2	169
81	Comparison of drive currents in metal-oxide-semiconductor field-effect transistors made of Si, Ge, GaAs, InGaAs, and InAs channels. Applied Physics Letters, 2010, 96, .	3.3	69
82	Phase diagram of Sr on Si(001): A first-principles study. Physical Review B, 2009, 80, .	3.2	33
83	Fundamental asymmetry in interfacial electronic reconstruction between insulating oxides: Anab initiostudy. Physical Review B, 2009, 79, .	3.2	53
84	Atomic Structure of the Epitaxial<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mi>BaO</mml:mi><mml:mo>/</mml:mo><mml:mi>Si</mml:mi><mml:mo stretchy="false">(</mml:mo><mml:mn>001</mml:mn><mml:mo) Tj ETQq0 0 0 rgBT /Overlock 10 Tf 50 292 Td (stretchy="false">)</mm	7.8	45
85	Diffraction studies of submonolayer Sr structures on the Si (001) surface. Journal of Vacuum Science & Technology B, 2009, 27, 2015.	1.3	7
86	Self-doping in boron sheets from first principles: A route to structural design of metal boride nanostructures. Physical Review B, 2009, 80, .	3.2	145
87	Electronic excitations in single-walled GaN nanotubes from first principles: Dark excitons and unconventional diameter dependences. Physical Review B, 2008, 77, .	3.2	41
88	Role of Strontium in Oxide Epitaxy on Silicon (001). Physical Review Letters, 2008, 101, 105503.	7.8	64
89	Quasiparticle and Excitonic Effects in the Optical Response of Nanotubes and Nanoribbons. Topics in Applied Physics, 2007, , 195-227.	0.8	22
90	Excited-state forces within time-dependent density-functional theory: A frequency-domain approach. Physical Review A, 2007, 76, .	2.5	17

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91	Novel Precursors for Boron Nanotubes: The Competition of Two-Center and Three-Center Bonding in Boron Sheets. Physical Review Letters, 2007, 99, 115501.	7.8	751
92	Excitons in carbon nanotubes: Diameter and chirality trends. Physica Status Solidi (B): Basic Research, 2007, 244, 4016-4020.	1.5	35
93	Truncation of periodic image interactions for confined systems. Physical Review B, 2006, 73, .	3.2	273
94	First principles calculation of optical and electronic properties with inclusion of exciton effects. Physica Status Solidi C: Current Topics in Solid State Physics, 2006, 3, 3365-3372.	0.8	5
95	Diameter and chirality dependence of exciton properties in carbon nanotubes. Physical Review B, 2006, 74, .	3.2	179
96	Selection rules for one- and two-photon absorption by excitons in carbon nanotubes. Physical Review B, 2006, 73, .	3.2	48
97	Self-Trapped Excitons in Silicon Dioxide: Mechanism and Properties. Physical Review Letters, 2005, 95, 156401.	7.8	93
98	Photoisomerization of azobenzene from first-principles constrained density-functional calculations. Journal of Chemical Physics, 2005, 122, 094311.	3.0	116
99	Theory andAbÂInitioCalculation of Radiative Lifetime of Excitons in Semiconducting Carbon Nanotubes. Physical Review Letters, 2005, 95, 247402.	7.8	295
100	Effect of semicore orbitals on the electronic band gaps of Si, Ge, and GaAs within the GW approximation. Physical Review B, 2004, 69, .	3.2	125
101	Excitonic Effects and Optical Spectra of Single-Walled Carbon Nanotubes. Physical Review Letters, 2004, 92, 077402.	7.8	875
102	Quasiparticle energies, excitonic effects and optical absorption spectra of small-diameter single-walled carbon nanotubes. Applied Physics A: Materials Science and Processing, 2004, 78, 1129-1136.	2.3	139
103	Excited-State Forces within a First-Principles Greenâ€™s Function Formalism. Physical Review Letters, 2003, 90, 076401.	7.8	97
104	Ab initioand finite-temperature molecular dynamics studies of lattice resistance in tantalum. Physical Review B, 2003, 68, .	3.2	44
105	Elasticity of nanometer-sized objects. Physical Review B, 2002, 65, .	3.2	46
106	Quasiparticle band structure of ZnS and ZnSe. Physical Review B, 2002, 66, .	3.2	99
107	Coupling of Nonlocal Potentials to Electromagnetic Fields. Physical Review Letters, 2001, 87, 087402.	7.8	56
108	New algebraic formulation of density functional calculation. Computer Physics Communications, 2000, 128, 1-45.	7.5	89

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109	New physics of the 30Â° partial dislocation in silicon revealed throughab initiocalculation. Journal of Physics Condensed Matter, 2000, 12, 10029-10037.	1.8	6
110	Ab InitioStudy of Screw Dislocations in Mo and Ta: A New Picture of Plasticity in bcc Transition Metals. Physical Review Letters, 2000, 84, 1499-1502.	7.8	185
111	Locality of the Density Matrix in Metals, Semiconductors, and Insulators. Physical Review Letters, 1999, 82, 2127-2130.	7.8	198
112	Edge-driven transition in the surface structure of nanoscale silicon. Physical Review B, 1998, 57, 11923-11926.	3.2	47
113	Paramagnetic Structure of the Soliton of the 30Â° Partial Dislocation in Silicon. Physical Review Letters, 1998, 80, 3984-3987.	7.8	20
114	Free energy of the concerted-exchange mechanism for self-diffusion in silicon. Physical Review B, 1996, 53, 1310-1314.	3.2	13