Sohrab Ismail-Beigi

List of Publications by Year
in descending order

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	Excitonic Effects and Optical Spectra of Single-Walled Carbon Nanotubes. Physical Review Letters, 2004, 92, 077402.	7.8	875
2	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
3	Theory andAbÂInitioCalculation of Radiative Lifetime of Excitons in Semiconducting Carbon Nanotubes. Physical Review Letters, 2005, 95, 247402.	7.8	295
4	Large-area single-crystal sheets of borophene on Cu(111) surfaces. Nature Nanotechnology, 2019, 14, 44-49.	31.5	285
5	Truncation of periodic image interactions for confined systems. Physical Review B, 2006, 73, .	3.2	273
6	Crystalline Oxides on Silicon. Advanced Materials, 2010, 22, 2919-2938.	21.0	203
7	Locality of the Density Matrix in Metals, Semiconductors, and Insulators. Physical Review Letters, 1999, 82, 2127-2130.	7.8	198
8	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
9	Diameter and chirality dependence of exciton properties in carbon nanotubes. Physical Review B, 2006, 74, .	3.2	179
10	First-principles study of boron sheets and nanotubes. Physical Review B, 2010, 82, .	3.2	169
11	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
12	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
13	Orbital Engineering in Symmetry-Breaking Polar Heterostructures. Physical Review Letters, 2015, 114, 026801.	7.8	135
14	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
15	Ferroelectric-Based Catalysis: Switchable Surface Chemistry. ACS Catalysis, 2015, 5, 4537-4545.	11.2	122
16	Photoisomerization of azobenzene from first-principles constrained density-functional calculations. Journal of Chemical Physics, 2005, 122, 094311.	3.0	116
17	Ferroelectrics: A pathway to switchable surface chemistry and catalysis. Surface Science, 2016, 650, 302-316.	1.9	114
18	Electronic and Magnetic Properties of SrTiO₃/LaAlO₃ Interfaces from First Principles. Advanced Materials, 2010, 22, 2881-2899.	21.0	107

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19	Quasiparticle band structure of ZnS and ZnSe. Physical Review B, 2002, 66, .	3.2	99
20	Tuning the Structure of Nickelates to Achieve Twoâ€Đimensional Electron Conduction. Advanced Materials, 2014, 26, 1935-1940.	21.0	99
21	Ferroelectric oxide surface chemistry: water splitting via pyroelectricity. Journal of Materials Chemistry A, 2016, 4, 5235-5246.	10.3	99
22	Excited-State Forces within a First-Principles Greenâ€™s Function Formalism. Physical Review Letters, 2003, 90, 076401.	7.8	97
23	LaTiO3/KTaO3 interfaces: A new two-dimensional electron gas system. APL Materials, 2015, 3, .	5.1	94
24	Self-Trapped Excitons in Silicon Dioxide: Mechanism and Properties. Physical Review Letters, 2005, 95, 156401.	7.8	93
25	New algebraic formulation of density functional calculation. Computer Physics Communications, 2000, 128, 1-45.	7.5	89
26	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
27	Chemistry of Ferroelectric Surfaces. Advanced Materials, 2010, 22, 2969-2973.	21.0	86
28	Alkaline earth stannates: The next silicon?. APL Materials, 2015, 3, 062510.	5.1	71
29	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
30	Modifying the Electronic Orbitals of Nickelate Heterostructures via Structural Distortions. Physical Review Letters, 2013, 110, 186402.	7.8	69
31	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
32	Polarization-driven catalysis via ferroelectric oxide surfaces. Physical Chemistry Chemical Physics, 2016, 18, 19676-19695.	2.8	65
33	Role of Strontium in Oxide Epitaxy on Silicon (001). Physical Review Letters, 2008, 101, 105503.	7.8	64
34	Reversible Modulation of Orbital Occupations via an Interface-Induced Polar State in Metallic Manganites. Nano Letters, 2014, 14, 4965-4970.	9.1	61
35	Coupling of Nonlocal Potentials to Electromagnetic Fields. Physical Review Letters, 2001, 87, 087402.	7.8	56
36	Causes of ferroelectricity in HfO₂-based thin films: an ab initio perspective. Physical Chemistry Chemical Physics, 2019, 21, 12150-12162.	2.8	56

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37	Fundamental asymmetry in interfacial electronic reconstruction between insulating oxides: Anab initiostudy. Physical Review B, 2009, 79, .	3.2	53
38	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
39	Selection rules for one- and two-photon absorption by excitons in carbon nanotubes. Physical Review B, 2006, 73, .	3.2	48
40	Edge-driven transition in the surface structure of nanoscale silicon. Physical Review B, 1998, 57, 11923-11926.	3.2	47
41	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></ Physical Review B, 2015, 92, .	3.2	47
42	Elasticity of nanometer-sized objects. Physical Review B, 2002, 65, .	3.2	46
43	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 ETQq1 1 0.784314 rgBT /Overlock 10 Tf 50 492 Td (stretchy="fa	7.8	45
44	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:< Physical Review Applied, 2014, 2, .	3.8	45
45	Ab initioand finite-temperature molecular dynamics studies of lattice resistance in tantalum. Physical Review B, 2003, 68, .	3.2	44
46	First-principles study of electronic reconstructions ofLaAlO3/SrTiO3heterointerfaces and their variants. Physical Review B, 2010, 82, .	3.2	44
47	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:mi></ System?. Physical Review Letters, 2017, 119, 067004.	7.8	44
48	Accurate tight-binding Hamiltonian matrices fromab initiocalculations: Minimal basis sets. Physical Review B, 2016, 93, .	3.2	43
49	Nature of Lone-Pairâ€“Surface Bonds and Their Scaling Relations. Inorganic Chemistry, 2018, 57, 7222-7238.	4.0	43
50	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:m xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mrow /><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:mrow	3.2	42
51	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
52	Picoscale materials engineering. Nature Reviews Materials, 2017, 2, .	48.7	42
53	Designing and controlling the properties of transition metal oxide quantum materials. Nature Materials, 2021, 20, 1462-1468.	27.5	42
54	Electronic excitations in single-walled GaN nanotubes from first principles: Dark excitons and unconventional diameter dependences. Physical Review B, 2008, 77, .	3.2	41

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55	Conduction at a Ferroelectric Interface. Physical Review Applied, 2014, 2, .	3.8	41
56	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	3.2	40
57	Dynamical 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> Physical Review Letters, 2011, 107, 105501.	7.8	38
58	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
59	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
60	Directing the Structure of Two-Dimensional Silica and Silicates. Journal of Physical Chemistry C, 2016, 120, 26770-26781.	3.1	36
61	Excitons in carbon nanotubes: Diameter and chirality trends. Physica Status Solidi (B): Basic Research, 2007, 244, 4016-4020.	1.5	35
62	Research Update: Orbital polarization in LaNiO₃-based heterostructures. APL Materials, 2015, 3, 062303.	5.1	34
63	Phase diagram of Sr on Si(001): A first-principles study. Physical Review B, 2009, 80, .	3.2	33
64	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:m Physical Review B, 2010, 81, .	3.2	31
65	Micrometre-scale single-crystalline borophene on a square-lattice Cu(100) surface. Nature Chemistry, 2022, 14, 377-383.	13.6	28
66	Single Atomic Layer Ferroelectric on Silicon. Nano Letters, 2018, 18, 241-246.	9.1	26
67	Intrinsic interfacial phenomena in manganite heterostructures. Journal of Physics Condensed Matter, 2015, 27, 123001.	1.8	25
68	Quasiparticle and Excitonic Effects in the Optical Response of Nanotubes and Nanoribbons. Topics in Applied Physics, 2007, , 195-227.	0.8	22
69	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
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	Paramagnetic Structure of the Soliton of the 30Â° Partial Dislocation in Silicon. Physical Review Letters, 1998, 80, 3984-3987.	7.8	20
72	Mechanism for strong binding of CdSe quantum dots to multiwall carbon nanotubes for solar energy harvesting. Nanoscale, 2013, 5, 6893.	5.6	18

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73	Excited-state forces within time-dependent density-functional theory: A frequency-domain approach. Physical Review A, 2007, 76, .	2.5	17
74	Controlling Mobility in Perovskite Oxides by Ferroelectric Modulation of Atomic-Scale Interface Structure. Nano Letters, 2018, 18, 573-578.	9.1	17
75	Complex-time shredded propagator method for large-scale <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:mi>G</mml:mi><mml:mi>W</mml:mi></mml:mrow></mm calculations. Physical Review B, 2020, 101, .	3.2	17
76	Generalized slave-particle method for extended Hubbard models. Physical Review B, 2015, 92, .	3.2	15
77	Justifying quasiparticle self-consistent schemes via gradient optimization in Baymâ€“Kadanoff theory. Journal of Physics Condensed Matter, 2017, 29, 385501.	1.8	15
78	Theory of Ferroelectric ZrO₂ Monolayers on Si. Journal of Physical Chemistry C, 2019, 123, 14350-14361.	3.1	15
79	Strong Orbital Polarization in a Cobaltate-Titanate Oxide Heterostructure. Physical Review Letters, 2019, 123, 117201.	7.8	14
80	Free energy of the concerted-exchange mechanism for self-diffusion in silicon. Physical Review B, 1996, 53, 1310-1314.	3.2	13
81	Surface Piezoelectricity of (0001) Sapphire. Physical Review Applied, 2019, 11, .	3.8	13
82	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
83	Growth and interfacial properties of epitaxial oxides on semiconductors: ab initio insights. Journal of Materials Science, 2012, 47, 7417-7438.	3.7	12
84	Imaging the buried MgO/Ag interface: Formation mechanism of the STM contrast. Physical Review B, 2014, 90, .	3.2	12
85	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:mn><m interface. Physical Review B, 2017, 96, .	3.2	11
86	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
87	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
88	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
89	Structure of a Two-Dimensional Silicate Layer Formed by Reaction with an Alloy Substrate. Chemistry of Materials, 2019, 31, 851-861.	6.7	11
90	Magnetism and piezoelectricity in stable transition metal silicate monolayers. Physical Review Materials, 2021, 5, .	2.4	10

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91	Phase transition of Sr on Si (001): First principles prediction and experiment. Surface Science, 2010, 604, 857-861.	1.9	9
92	Scalable GW software for quasiparticle properties using OpenAtom. Computer Physics Communications, 2019, 244, 427-441.	7.5	9
93	Revealing surface-state transport in ultrathin topological crystalline insulator SnTe films. APL Materials, 2019, 7, .	5.1	9
94	Symmetry breaking in occupation number based slave-particle methods. Physical Review B, 2017, 96, .	3.2	8
95	Diffraction studies of submonolayer Sr structures on the Si (001) surface. Journal of Vacuum Science & Technology B, 2009, 27, 2015.	1.3	7
96	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
109	Degree of locality of elasto-optic response in solids. Physical Review B, 2019, 100, .	3.2	2
110	Experimental and theoretical investigation of the formation of two-dimensional Fe silicate on Pd(111). Journal of Vacuum Science and Technology A: Vacuum, Surfaces and Films, 2021, 39, .	2.1	2
111	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
112	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
113	Identifying crystal structures and chemical reactions at the interface of stanene on Bi2Te3. Journal of Applied Physics, 2020, 128, .	2.5	1
114	Epitaxial binding and strain effects of monolayer stanene on the Al2O3(0001) surface. Physical Review Materials, 2022, 6, .	2.4	0