Sohrab Ismail-Beigi

List of Publications by Year in Descending Order

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	Micrometre-scale single-crystalline borophene on a square-lattice Cu(100) surface.. *Nature Chemistry*, **2022**,	17.6	2
107	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, 062201	2.9	0
106	Origin of the orbital polarization of Co2+ in La2CoTiO6 and (LaCoO3)1+(LaTiO3)1: A DFT+U and DFMT study. *Physical Review B*, **2021**, 103,	3.3	2
105	Designing and controlling the properties of transition metal oxide quantum materials. *Nature Materials*, **2021**, 20, 1462-1468	27	8
104	Boson Subsidiary Solver (BoSS) v1.1. *Computer Physics Communications*, **2021**, 265, 107991	4.2	1
103	Complex-time shredded propagator method for large-scale GW calculations. *Physical Review B*, **2020**, 101,	3.3	9
102	Magnetism of (LaCoO3)n+(LaTiO3)n superlattices (n=1,2). *Physical Review B*, **2020**, 101,	3.3	3
101	Identifying crystal structures and chemical reactions at the interface of stanene on Bi2Te3. *Journal of Applied Physics*, **2020**, 128, 165301	2.5	
100	Strong Orbital Polarization in a Cobaltate-Titanate Oxide Heterostructure. *Physical Review Letters*, **2019**, 123, 117201	7.4	9
99	Growth of ultrathin Ru oxide films on perovskite and corundum substrates. *Surface Science*, **2019**, 688, 51-62	1.8	2
98	Ferroelectric ZrO2 Monolayers as Buffer Layers between SrTiO3 and Si. *Journal of Physical Chemistry C*, **2019**, 123, 15053-15061	3.8	2
97	Scalable GW software for quasiparticle properties using OpenAtom. *Computer Physics Communications*, **2019**, 244, 427-441	4.2	4
96	Theory of Ferroelectric ZrO2 Monolayers on Si. *Journal of Physical Chemistry C*, **2019**, 123, 14350-14361	3.8	9
95	Revealing surface-state transport in ultrathin topological crystalline insulator SnTe films. *APL Materials*, **2019**, 7, 051106	5.7	6
94	Causes of ferroelectricity in HfO-based thin films: an ab initio perspective. *Physical Chemistry Chemical Physics*, **2019**, 21, 12150-12162	3.6	34
93	Surface Piezoelectricity of (0001) Sapphire. *Physical Review Applied*, **2019**, 11,	4.3	7
92	Tuning two-dimensional phase formation through epitaxial strain and growth conditions: silica and silicate on NiPd(111) alloy substrates. *Nanoscale*, **2019**, 11, 21340-21353	7.7	5

91	Structure of a Two-Dimensional Silicate Layer Formed by Reaction with an Alloy Substrate. *Chemistry of Materials*, **2019**, 31, 851-861	9.6	4
90	Large-area single-crystal sheets of borophene on Cu(111) surfaces. *Nature Nanotechnology*, **2019**, 14, 44-49	28.7	171
89	Controlling Mobility in Perovskite Oxides by Ferroelectric Modulation of Atomic-Scale Interface Structure. *Nano Letters*, **2018**, 18, 573-578	11.5	8
88	Nature of Lone-Pair-Surface Bonds and Their Scaling Relations. *Inorganic Chemistry*, **2018**, 57, 7222-7238	5.1	35
87	Suppression of the spectral weight of topological surface states on the nanoscale via local symmetry breaking. *Physical Review Materials*, **2018**, 2,	3.2	3
86	Two-dimensional electron gas oxide remote doping of Si(001). *Physical Review Materials*, **2018**, 2,	3.2	6
85	Single Atomic Layer Ferroelectric on Silicon. *Nano Letters*, **2018**, 18, 241-246	11.5	16
84	Length Scale and Dimensionality of Defects in Epitaxial SnTe Topological Crystalline Insulator Films. *Advanced Materials Interfaces*, **2017**, 4, 1601011	4.6	5
83	Picoscale materials engineering. *Nature Reviews Materials*, **2017**, 2,	73.3	33
82	Ab initio study of the BaTiO3/Ge interface. *Physical Review B*, **2017**, 96,	3.3	10
81	How Correlated is the FeSe/SrTiO_{3} System?. *Physical Review Letters*, **2017**, 119, 067004	7.4	34
80	Symmetry breaking in occupation number based slave-particle methods. *Physical Review B*, **2017**, 96,	3.3	2
79	Justifying quasiparticle self-consistent schemes via gradient optimization in Baym-Kadanoff theory. *Journal of Physics Condensed Matter*, **2017**, 29, 385501	1.8	4
78	Experimental verification of orbital engineering at the atomic scale: Charge transfer and symmetry breaking in nickelate heterostructures. *Physical Review B*, **2017**, 95,	3.3	9
77	Control of hidden ground-state order in NdNiO3 superlattices. *Physical Review Materials*, **2017**, 1,	3.2	9
76	Accurate tight-binding Hamiltonian matrices from ab initio calculations: Minimal basis sets. *Physical Review B*, **2016**, 93,	3.3	29
75	Role of double TiO2 layers at the interface of FeSe/SrTiO3 superconductors. *Physical Review B*, **2016**, 93,	3.3	35
74	Charge transfer and negative curvature energy in magnesium boride nanotubes. *Physical Review B*, **2016**, 94,	3.3	2

73	Directing the Structure of Two-Dimensional Silica and Silicates. *Journal of Physical Chemistry C*, **2016**, 120, 26770-26781	3.8	28
72	Ferroelectric oxide surface chemistry: water splitting via pyroelectricity. *Journal of Materials Chemistry A*, **2016**, 4, 5235-5246	13	78
71	Ferroelectrics: A pathway to switchable surface chemistry and catalysis. *Surface Science*, **2016**, 650, 302-316	2.6	94
70	Polarization-driven catalysis via ferroelectric oxide surfaces. *Physical Chemistry Chemical Physics*, **2016**, 18, 19676-95	3.6	55
69	Intrinsic interfacial phenomena in manganite heterostructures. *Journal of Physics Condensed Matter* , **2015**, 27, 123001	1.8	22
68	Ferroelectric-Based Catalysis: Switchable Surface Chemistry. *ACS Catalysis*, **2015**, 5, 4537-4545	13.1	90
67	LaTiO3/KTaO3 interfaces: A new two-dimensional electron gas system. *APL Materials*, **2015**, 3, 036104	5.7	60
66	Alkaline earth stannates: The next silicon?. *APL Materials*, **2015**, 3, 062510	5.7	61
65	First-principles study of oxygen-deficient LaNiO3 structures. *Physical Review B*, **2015**, 92,	3.3	26
64	Generalized slave-particle method for extended Hubbard models. *Physical Review B*, **2015**, 92,	3.3	10
63	Importance of anisotropic Coulomb interaction in LaMnO3. *Physical Review B*, **2015**, 92,	3.3	35
62	Research Update: Orbital polarization in LaNiO3-based heterostructures. *APL Materials*, **2015**, 3, 062303	5.7	27
61	Orbital engineering in symmetry-breaking polar heterostructures. *Physical Review Letters*, **2015**, 114, 026801	7.4	109
60	Tuning the structure of nickelates to achieve two-dimensional electron conduction. *Advanced Materials*, **2014**, 26, 1935-40	24	81
59	Controlled doping of carbon nanotubes with metallocenes for application in hybrid carbon nanotube/Si solar cells. *Nano Letters*, **2014**, 14, 3388-94	11.5	45
58	Reversible modulation of orbital occupations via an interface-induced polar state in metallic manganites. *Nano Letters*, **2014**, 14, 4965-70	11.5	58
57	Imaging the buried MgO/Ag interface: Formation mechanism of the STM contrast. *Physical Review B* , **2014**, 90,	3.3	9
56	Effect of Surface Termination on the Electronic Properties of LaNiO3 Films. *Physical Review Applied*, **2014**, 2,	4.3	34

55	Formation and atomic structure of ordered Sr-induced nanostrips on Ge(100). *Physical Review B*, **2014**, 89,	3.3	6
54	Conduction at a Ferroelectric Interface. *Physical Review Applied*, **2014**, 2,	4.3	37
53	Modifying the electronic orbitals of nickelate heterostructures via structural distortions. *Physical Review Letters*, **2013**, 110, 186402	7.4	59
52	Mechanism for strong binding of CdSe quantum dots to multiwall carbon nanotubes for solar energy harvesting. *Nanoscale*, **2013**, 5, 6893-900	7.7	18
51	Ferroelectric surface chemistry: First-principles study of the PbTiO3 surface. *Physical Review B*, **2013**, 88,	3.3	77
50	Directed self-assembly of hybrid oxide/polymer core/shell nanowires with transport optimized morphology for photovoltaics. *Advanced Materials*, **2012**, 24, 82-7	24	35
49	Growth and interfacial properties of epitaxial oxides on semiconductors: ab initio insights. *Journal of Materials Science*, **2012**, 47, 7417-7438	4.3	11
48	Ferroelectric control of magnetization in La1⊠SrxMnO3 manganites: A first-principles study. *Physical Review B*, **2012**, 86,	3.3	42
47	Interface structure and film polarization in epitaxial SrTiO3/Si(001). *Physical Review B*, **2012**, 85,	3.3	31
46	Deciphering the atomic structure of a complex Sr/Ge (100) phase via scanning tunneling microscopy and first-principles calculations. *Physical Review B*, **2012**, 85,	3.3	12
45	Thermodynamic stability and growth kinetics of epitaxial SrTiO3 on silicon. *Physical Review B*, **2011**, 83,	3.3	21
44	Dynamic evanescent phonon coupling across the La(1-x)Sr(x)MnO3/SrTiO3 interface. *Physical Review Letters*, **2011**, 107, 105501	7.4	31
43	Correlation energy functional within the GW-RPA: Exact forms, approximate forms, and challenges. *Physical Review B*, **2010**, 81,	3.3	20
42	Interface-induced polarization and inhibition of ferroelectricity in epitaxial SrTiO⁄Si. *Physical Review Letters*, **2010**, 105, 217601	7.4	62
41	Electric field tuned crossover from classical to weakly localized quantum transport in electron doped SrTiO3. *Physical Review B*, **2010**, 81,	3.3	28
40	First-principles study of electronic reconstructions of LaAlO3/SrTiO3 heterointerfaces and their variants. *Physical Review B*, **2010**, 82,	3.3	35
39	First-principles study of boron sheets and nanotubes. *Physical Review B*, **2010**, 82,	3.3	144
38	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, 122105	3.4	55

37	Chemistry of ferroelectric surfaces. *Advanced Materials*, **2010**, 22, 2969-73	24	76
36	Electronic and magnetic properties of SrTiO(3)/LaAlO(3) interfaces from first principles. *Advanced Materials*, **2010**, 22, 2881-99	24	95
35	Crystalline oxides on silicon. *Advanced Materials*, **2010**, 22, 2919-38	24	180
34	Phase transition of Sr on Si (001): First principles prediction and experiment. *Surface Science*, **2010**, 604, 857-861	1.8	9
33	Phase diagram of Sr on Si(001): A first-principles study. *Physical Review B*, **2009**, 80,	3.3	31
32	Fundamental asymmetry in interfacial electronic reconstruction between insulating oxides: An ab initio study. *Physical Review B*, **2009**, 79,	3.3	51
31	Atomic structure of the epitaxial BaO/Si(001) interface. *Physical Review Letters*, **2009**, 102, 116101	7.4	42
30	Diffraction studies of submonolayer Sr structures on the Si (001) surface. *Journal of Vacuum Science & Technology B*, **2009**, 27, 2015		7
29	Self-doping in boron sheets from first principles: A route to structural design of metal boride nanostructures. *Physical Review B*, **2009**, 80,	3.3	124
28	Electronic excitations in single-walled GaN nanotubes from first principles: Dark excitons and unconventional diameter dependences. *Physical Review B*, **2008**, 77,	3.3	38
27	Role of strontium in oxide epitaxy on silicon (001). *Physical Review Letters*, **2008**, 101, 105503	7.4	59
26	Novel precursors for boron nanotubes: the competition of two-center and three-center bonding in boron sheets. *Physical Review Letters*, **2007**, 99, 115501	7.4	629
25	Excitons in carbon nanotubes: Diameter and chirality trends. *Physica Status Solidi (B): Basic Research* , **2007**, 244, 4016-4020	1.3	29
24	Quasiparticle and Excitonic Effects in the Optical Response of Nanotubes and Nanoribbons. *Topics in Applied Physics*, **2007**, 195-227	0.5	17
23	Excited-state forces within time-dependent density-functional theory: A frequency-domain approach. *Physical Review A*, **2007**, 76,	2.6	17
22	Truncation of periodic image interactions for confined systems. *Physical Review B*, **2006**, 73,	3.3	207
21	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		4
20	Diameter and chirality dependence of exciton properties in carbon nanotubes. *Physical Review B*, **2006**, 74,	3.3	168

19	Selection rules for one- and two-photon absorption by excitons in carbon nanotubes. *Physical Review B*, **2006**, 73,	3.3	43
18	Photoisomerization of azobenzene from first-principles constrained density-functional calculations. *Journal of Chemical Physics*, **2005**, 122, 094311	3.9	108
17	Theory and ab initio calculation of radiative lifetime of excitons in semiconducting carbon nanotubes. *Physical Review Letters*, **2005**, 95, 247402	7.4	248
16	Self-trapped excitons in silicon dioxide: mechanism and properties. *Physical Review Letters*, **2005**, 95, 156401	7.4	79
15	Effect of semicore orbitals on the electronic band gaps of Si, Ge, and GaAs within the GW approximation. *Physical Review B*, **2004**, 69,	3.3	114
14	Excitonic effects and optical spectra of single-walled carbon nanotubes. *Physical Review Letters*, **2004**, 92, 077402	7.4	805
13	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	2.6	126
12	Excited-state forces within a first-principles Green function formalism. *Physical Review Letters*, **2003**, 90, 076401	7.4	84
11	Ab initio and finite-temperature molecular dynamics studies of lattice resistance in tantalum. *Physical Review B*, **2003**, 68,	3.3	42
10	Elasticity of nanometer-sized objects. *Physical Review B*, **2002**, 65,	3.3	43
9	Quasiparticle band structure of ZnS and ZnSe. *Physical Review B*, **2002**, 66,	3.3	92
8	Coupling of nonlocal potentials to electromagnetic fields. *Physical Review Letters*, **2001**, 87, 087402	7.4	51
7	New algebraic formulation of density functional calculation. *Computer Physics Communications*, **2000**, 128, 1-45	4.2	78
6	New physics of the 30°partial dislocation in silicon revealed throughab initiocalculation. *Journal of Physics Condensed Matter*, **2000**, 12, 10029-10037	1.8	2
5	Ab initio study of screw dislocations in Mo and ta: A new picture of plasticity in bcc transition metals. *Physical Review Letters*, **2000**, 84, 1499-502	7.4	172
4	Locality of the Density Matrix in Metals, Semiconductors, and Insulators. *Physical Review Letters*, **1999**, 82, 2127-2130	7.4	164
3	Edge-driven transition in the surface structure of nanoscale silicon. *Physical Review B*, **1998**, 57, 11923-11926	3.3	47
2	Paramagnetic Structure of the Soliton of the 30°Partial Dislocation in Silicon. *Physical Review Letters*, **1998**, 80, 3984-3987	7.4	17

1 Free energy of the concerted-exchange mechanism for self-diffusion in silicon. *Physical Review B*, **1996**, 53, 1310-1314 3.3 12