

# Kevin F Garrity

## List of Publications by Year in descending order

Source: <https://exaly.com/author-pdf/7306611/publications.pdf>

Version: 2024-02-01

32  
papers

3,927  
citations

304743

22  
h-index

434195

31  
g-index

34  
all docs

34  
docs citations

34  
times ranked

6336  
citing authors

#	ARTICLE	IF	CITATIONS
1	Pseudopotentials for high-throughput DFT calculations. Computational Materials Science, 2014, 81, 446-452.	3.0	1,114
2	Reproducibility in density functional theory calculations of solids. Science, 2016, 351, aad3000.	12.6	1,113
3	Antiferroelectricity in thin-film $ZrO_2$ from first principles. Physical Review B, 2014, 90, .	3.2	205
4	Crystalline Oxides on Silicon. Advanced Materials, 2010, 22, 2919-2938.	21.0	203
5	The joint automated repository for various integrated simulations (JARVIS) for data-driven materials design. Npj Computational Materials, 2020, 6, .	8.7	181
6	Wannier center sheets in topological insulators. Physical Review B, 2014, 89, .	3.2	139
7	Hexagonal $ABC$ Semiconductors as Ferroelectrics. Physical Review Letters, 2012, 109, 167602.	7.8	114
8	Chern Insulators from Heavy Atoms on Magnetic Substrates. Physical Review Letters, 2013, 110, 116802.	7.8	99
9	Hyperferroelectrics: Proper Ferroelectrics with Persistent Polarization. Physical Review Letters, 2014, 112, 127601.	7.8	76
10	High-throughput density functional perturbation theory and machine learning predictions of infrared, piezoelectric, and dielectric responses. Npj Computational Materials, 2020, 6, .	8.7	60
11	Orthorhombic $ABC$ Semiconductors as Antiferroelectrics. Physical Review Letters, 2013, 110, 017603.	7.8	59
12	Distinct magneto-Raman signatures of spin-flip phase transitions in CrI <sub>3</sub> . Nature Communications, 2020, 11, 3879.	12.8	59
13	Chern insulator at a magnetic rocksalt interface. Physical Review B, 2014, 90, .	3.2	47
14	Prediction of Weyl semimetal and antiferromagnetic topological insulator phases in Bi <sub>2</sub> MnSe <sub>4</sub> . Npj Computational Materials, 2019, 5, .	8.7	47
15	Intertwined Rashba, Dirac, and Weyl Fermions in Hexagonal Hyperferroelectrics. Physical Review Letters, 2016, 117, 076401.	7.8	42
16	Data-driven discovery of 3D and 2D thermoelectric materials. Journal of Physics Condensed Matter, 2020, 32, 475501.	1.8	42
17	First-principles search for $n$ -type oxide, nitride, and sulfide thermoelectrics. Physical Review B, 2016, 94, .	3.2	39
18	Flux States and Topological Phases from Spontaneous Time-Reversal Symmetry Breaking in $CrSiGe$ Systems. Physical Review Letters, 2016, 117, 257201.	7.8	37

#	ARTICLE	IF	CITATIONS
19	High-throughput Discovery of Topologically Non-trivial Materials using Spin-orbit Spillage. Scientific Reports, 2019, 9, 8534.	3.3	36
20	Magnon-phonon hybridization in 2D antiferromagnet MnPSe <sub>3</sub> . Science Advances, 2021, 7, eabj3106.	10.3	35
21	High-throughput first-principles search for new ferroelectrics. Physical Review B, 2018, 97, .	3.2	33
22	Computational search for magnetic and non-magnetic 2D topological materials using unified spin-orbit spillage screening. Npj Computational Materials, 2020, 6, .	8.7	32
23	High-throughput search for magnetic topological materials using spin-orbit spillage, machine learning, and experiments. Physical Review B, 2021, 103, .	3.2	22
24	Database of Wannier tight-binding Hamiltonians using high-throughput density functional theory. Scientific Data, 2021, 8, 106.	5.3	20
25	Topological surface states of $Mn_2Bi$ at finite temperatures and at domain walls. Physical Review Materials, 2021, 5, .		
26	Computational scanning tunneling microscope image database. Scientific Data, 2021, 8, 57.	5.3	15
27	Growth and interfacial properties of epitaxial oxides on semiconductors: ab initio insights. Journal of Materials Science, 2012, 47, 7417-7438.	3.7	12
28	Phase transition of Sr on Si (001): First principles prediction and experiment. Surface Science, 2010, 604, 857-861.	1.9	9
29	Effects of octahedral tilting on the site of substitution of manganese in CaTiO <sub>3</sub> . Acta Materialia, 2021, 207, 116688.	7.9	9
30	Formation and atomic structure of ordered Sr-induced nanostrips on Ge(100). Physical Review B, 2014, 89, .	3.2	6
31	Combined cluster and atomic displacement expansion for solid solutions and magnetism. Physical Review B, 2019, 99, .	3.2	5
32	Effects of Octahedral Tilting on the Site of Substitution of Manganese in CaTiO <sub>3</sub> . SSRN Electronic Journal, 0, , .	0.4	1