Manh Cuong Nguyen

List of Publications by Year in Descending Order

55 papers	1,161 citations	18 h-index	33 g-index
57 ext. papers	1,436 ext. citations	4 avg, IF	4.3 L-index

#	Paper	IF	Citations
55	Spatial decomposition of magnetic anisotropy in magnets: Application to doped Fe16N2. *Physical Review B*, **2020**, 102,	3.3	3
54	Thermophysical and mechanical properties of novel high-entropy metal nitride-carbides. *Journal of the American Ceramic Society*, **2020**, 103, 6475-6489	3.8	17
53	Adaptive Genetic Algorithm for Structure Prediction and Application to Magnetic Materials **2020**, 2757-2776		
52	Concentration-tuned tetragonal strain in alloys: Application to magnetic anisotropy of FeNi1−xCox. *Physical Review B*, **2019**, 100,	3.3	5
51	Single-Crystal Permanent Magnets: Extraordinary Magnetic Behavior in the Ta-, Cu-, and Fe-Substituted CeCo5 Systems. *Physical Review Applied*, **2019**, 11,	4.3	9
50	Quantum phase transition and ferromagnetism in Co1+xSn. *Physical Review B*, **2019**, 99,	3.3	4
49	First-principles study, fabrication and characterization of (Zr0.25Nb0.25Ti0.25V0.25)C high-entropy ceramics. *Acta Materialia*, **2019**, 170, 15-23	8.4	127
48	Adaptive Genetic Algorithm for Structure Prediction and Application to Magnetic Materials **2019**, 1-20		
47	Magnetocrystalline anisotropy in cobalt based magnets: a choice of correlation parameters and the relativistic effects. *Journal of Physics Condensed Matter*, **2018**, 30, 195801	1.8	14
46	New structures of Fe3S for rare-earth-free permanent magnets. *Journal Physics D: Applied Physics*, **2018**, 51, 075001	3	2
45	Fe-Si networks and charge/discharge-induced phase transitions in LiFeSiO cathode materials. *Physical Chemistry Chemical Physics*, **2018**, 20, 14557-14563	3.6	11
44	Using first-principles calculations to screen for fragile magnetism: Case study of LaCrGe3 and LaCrSb3. *Physical Review B*, **2018**, 97,	3.3	3
43	Structures and magnetic properties of iron silicide from adaptive genetic algorithm and first-principles calculations. *Journal of Applied Physics*, **2018**, 124, 073901	2.5	4
42	Magnetocrystalline anisotropy in YCo5 and ZrCo5 compounds from first-principles real-space pseudopotentials calculations. *Physical Review Materials*, **2018**, 2,	3.2	3
41	Prediction of novel stable Fe-V-Si ternary phase. *Journal of Alloys and Compounds*, **2018**, 732, 567-572	5.7	2
40	Electronic structure, optical and magnetic studies of PLD-grown (Mn, P)-doped ZnO nanocolumns at room temperature. *Journal Physics D: Applied Physics*, **2017**, 50, 295002	3	2
39	A scheme for the generation of FeP networks to search for low-energy LiFePO4 crystal structures. *Journal of Materials Chemistry A*, **2017**, 5, 14611-14618	13	9

38	Role of Surface Stress on the Reactivity of Anatase TiO(001). *Journal of Physical Chemistry Letters*, **2017**, 8, 1764-1771	6.4	29
37	Growth and characterization of BaZnGa. *Philosophical Magazine*, **2017**, 97, 3317-3324	1.6	
36	Structures of defects on anatase TiO(001) surfaces. *Nanoscale*, **2017**, 9, 11553-11565	7.7	17
35	Structures, phase transitions, and magnetic properties of Co3Si from first-principles calculations. *Physical Review B*, **2017**, 96,	3.3	6
34	Elastic and electronic tuning of magnetoresistance in MoTe. *Science Advances*, **2017**, 3, eaao4949	14.3	30
33	Cluster-Expansion Model for Complex Quinary Alloys: Application to Alnico Permanent Magnets. *Physical Review Applied*, **2017**, 8,	4.3	6
32	Crystal structure and magnetic properties of new Fe3Co3X2(X = Ti, Nb) intermetallic compounds. *Journal Physics D: Applied Physics*, **2016**, 49, 175002	3	4
31	Stabilities and defect-mediated lithium-ion conduction in a ground state cubic Li3N structure. *Physical Chemistry Chemical Physics*, **2016**, 18, 4185-90	3.6	4
30	Structure and magnetism of new rare-earth-free intermetallic compounds: Fe3+xCo3−xTi2 (0 ⩽ x ⩽ 3). *APL Materials*, **2016**, 4, 116109	5.7	3
29	Robust diamond-like Fe-Si network in the zero-strain Na FeSiO4 cathode. *Electrochimica Acta*, **2016**, 212, 934-940	6.7	27
28	Ferromagnetic Quantum Critical Point Avoided by the Appearance of Another Magnetic Phase in LaCrGe_{3} under Pressure. *Physical Review Letters*, **2016**, 117, 037207	7.4	23
27	Development of interatomic potentials appropriate for simulation of devitrification of Al90Sm10alloy. *Modelling and Simulation in Materials Science and Engineering*, **2015**, 23, 045013	2	43
26	Cluster expansion modeling and Monte Carlo simulation of alnico 5⁻7 permanent magnets. *Journal of Applied Physics*, **2015**, 117, 093905	2.5	5
25	Exploration of tetrahedral structures in silicate cathodes using a motif-network scheme. *Scientific Reports*, **2015**, 5, 15555	4.9	24
24	Structures and magnetic properties of Co-Zr-B magnets studied by first-principles calculations. *Journal of Applied Physics*, **2015**, 117, 243902	2.5	12
23	First-principles study of direct and narrow band gap semiconducting □CuGaO2. *Materials Research Express*, **2015**, 2, 045902	1.7	9
22	Fluctuation Hall Conductivity Beyond Linear Response in Layered Superconductors Under a Magnetic Field. *Journal of Superconductivity and Novel Magnetism*, **2014**, 27, 359-363	1.5	
21	Orthorhombic Zr2Co11 phase revisited. *Journal of Alloys and Compounds*, **2014**, 611, 167-170	5.7	5

20	sp3-hybridized framework structure of group-14 elements discovered by genetic algorithm. *Physical Review B*, **2014**, 89,	3.3	20
19	An adaptive genetic algorithm for crystal structure prediction. *Journal of Physics Condensed Matter*, **2014**, 26, 035402	1.8	75
18	New Be-intercalated hexagonal boron layer structure of BeB2. *RSC Advances*, **2014**, 4, 15061-15065	3.7	2
17	Interface Structure Prediction from First-Principles. *Journal of Physical Chemistry C*, **2014**, 118, 9524-9530	4.8	28
16	Exploring the structural complexity of intermetallic compounds by an adaptive genetic algorithm. *Physical Review Letters*, **2014**, 112, 045502	7.4	78
15	On-the-fly machine-learning for high-throughput experiments: search for rare-earth-free permanent magnets. *Scientific Reports*, **2014**, 4, 6367	4.9	160
14	New stable Re-B phases for ultra-hard materials. *Journal of Physics Condensed Matter*, **2014**, 26, 455401	1.8	5
13	Genetic algorithm prediction of crystal structure of metastable Si-IX phase. *Solid State Communications*, **2014**, 182, 14-16	1.6	6
12	New layered structures of cuprous chalcogenides as thin film solar cell materials: Cu2Te and Cu2Se. *Physical Review Letters*, **2013**, 111, 165502	7.4	88
11	Atomic Structure and Magnetic Properties of HfCo$_{7}$ Alloy. *IEEE Transactions on Magnetics*, **2013**, 49, 3281-3283	2	6
10	Structures and stabilities of alkaline earth metal peroxides XO2 (X = Ca, Be, Mg) studied by a genetic algorithm. *RSC Advances*, **2013**, 3, 22135	3.7	16
9	Atomic structure and magnetic properties of Fe1−xCox alloys. *Journal of Applied Physics*, **2012**, 111, 07E338	2.5	18
8	Calcium-decorated, hydroxylated single-walled carbon nanotubes for hydrogen storage: a first-principles study. *ChemPhysChem*, **2011**, 12, 777-80	3.2	4
7	SIMULTANEOUS DESCRIPTION OF STRONG AND WEAK H2 ADSORPTION SITES COEXISTING IN MOFs. *Nano*, **2011**, 06, 225-229	1.1	4
6	Iron-Decorated, Functionalized Metal Organic Framework for High-Capacity Hydrogen Storage: First-Principles Calculations. *Journal of Physical Chemistry C*, **2010**, 114, 14276-14280	3.8	25
5	Hydrogen storage in Ca-decorated, B-substituted metal organic framework. *International Journal of Hydrogen Energy*, **2010**, 35, 198-203	6.7	34
4	Calcium-hydroxyl group complex for potential hydrogen storage media: A density functional theory study. *Physical Review B*, **2009**, 79,	3.3	7
3	Titanium-functional group complexes for high-capacity hydrogen storage materials. *Solid State Communications*, **2008**, 146, 431-434	1.6	27

2	Hydrogen storage using functionalized saturated hydrocarbons. *Solid State Communications*, **2008**, 147, 419-422	1.6	13
1	Ab initio study of dihydrogen binding in metal-decorated polyacetylene for hydrogen storage. *Physical Review B*, **2007**, 76,	3.3	83