Phuti E Ngoepe

List of Publications by Year
in descending order

58 papers	1,136 citations	361413 20 h-index	414414 32 g-index
59 all docs	59 docs citations	59 times ranked	1369 citing authors

#	Article	IF	Citations
1	Predicting the Electrochemical Properties of MnO₂ Nanomaterials Used in Rechargeable Li Batteries: Simulating Nanostructure at the Atomistic Level. Journal of the American Chemical Society, 2009, 131, 6161-6173.	13.7	74
2	Modeling the Surface Structure and Reactivity of Pyrite:Â Introducing a Potential Model for FeS2. Journal of Physical Chemistry B, 2000, 104, 7969-7976.	2.6	72
3	Generating MnO2Nanoparticles Using Simulated Amorphization and Recrystallization. Journal of the American Chemical Society, 2005, 127, 12828-12837.	13.7	69
4	The Displacive Phase Transition of Vanadium Dioxide and the Effect of Doping with Tungsten. Chemistry of Materials, 2008, 20, 1764-1772.	6.7	68
5	Link between structural and mechanical stability of fcc- and bcc-based ordered Mgâ€“Li alloys. Intermetallics, 2010, 18, 2083-2089.	3.9	59
6	Lithium and oxygen adsorption at the Î²-MnO2 (110) surface. Journal of Materials Chemistry A, 2013, 1, 14879.	10.3	58
7	Behavior of elastic constants, refractive index, and lattice parameter of cubic zirconia at high temperatures. Journal of Applied Physics, 1993, 73, 7268-7274.	2.5	44
8	Solid-state transformation in nanocrystalline Ti induced by ball milling. Materials Letters, 2010, 64, 1215-1218.	2.6	41
9	Highâ€temperature elastic constants of yttrium aluminum garnet. Journal of Applied Physics, 1993, 73, 7298-7301.	2.5	39
10	Structural, elastic and electronic properties of equiatomic PtTi as potential high-temperature shape memory alloy. Intermetallics, 2013, 33, 27-32.	3.9	37
11	Theoretical investigation of the Pt3Al ground state. Intermetallics, 2010, 18, 417-421.	3.9	36
12	Atomistic simulation of the surface structure of electrolytic manganese dioxide. Surface Science, 2009, 603, 3184-3190.	1.9	32
13	Negative compressibility in platinum sulfide using density-functional theory. Physical Review B, 2010, 81, .	3.2	31
14	Adsorption mechanisms and effects of thiocarbamate collectors in the separation of chalcopyrite from pyrite minerals: DFT and experimental studies. Minerals Engineering, 2022, 176, 107318.	4.3	28
15	Brillouin-scattering and computer-simulation studies of fast-ion conductors: a review. Journal of the Chemical Society, Faraday Transactions, 1990, 86, 1183.	1.7	27
16	Atomistic simulation of the structure and elastic properties of pyrite (FeS 2) as a function of pressure. Physics and Chemistry of Minerals, 2003, 30, 615-619.	0.8	27
17	A computer modelling study of the interaction of organic adsorbates with fluorapatite surfaces. Physics and Chemistry of Minerals, 2006, 33, 314-331.	0.8	25
18	Ab initio calculation of the voltage profile for LiC6. Solid State Ionics, 2003, 159, 21-23.	2.7	24

#	Article	IF	Citations
19	Simulating Mechanical Deformation in Nanomaterials with Application for Energy Storage in Nanoporous Architectures. ACS Nano, 2009, 3, 3308-3314.	14.6	23
20	Ab initio investigation of the thermodynamics of cation distribution and of the electronic and magnetic structures in the <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:msub><mml:mi>LiMn</mml:mi><mml:mn>2</mml:mn></mml:msub><mml:msub><mml:mi mathvariant="normal">O</mml:mi><mml:mn>4</mml:mn></mml:msub></mml:mrow></mml:math> spinel. Physical Review B, 2018, 97, .	3.2	21
21	Calculated cell discharge curve for lithium batteries with a V2O5 cathode. Journal of Materials Chemistry, 2000, 10, 239-240.	6.7	20
22	Nanoscale coatings of AuAlx and PtAlx and their mesoporous elemental derivatives. Current Applied Physics, 2006, 6, 440-443.	2.4	20
23	Electronic Structure and Redox Properties of the Ti-Doped Zirconia (111) Surface. Journal of Physical Chemistry C, 2010, 114, 15403-15409.	3.1	20
24	Amorphization and recrystallization study of lithium insertion into manganese dioxide. Physical Chemistry Chemical Physics, 2011, 13, 1307-1313.	2.8	20
25	Origin of electrochemical activity in nano-Li₂MnO₃; stabilization via a â€˜point defect scaffoldâ€™. Nanoscale, 2015, 7, 1167-1180.	5.6	20
26	Thermodynamically accessible titanium clusters Ti_N, N = 2â€“32. Physical Chemistry Chemical Physics, 2018, 20, 13962-13973.	2.8	18
27	Ethylene carbonate adsorption on the major surfaces of lithium manganese oxide Li_{1â^'x}Mn₂O₄spinel (0.000 <<i>x</i>< 0.375): a DFT+<i>U</i>-D3 study. Physical Chemistry Chemical Physics, 2020, 22, 6763-6771.	2.8	18
28	An alternative DFT-based model for calculating structural and elastic properties of random binary HCP, FCC and BCC alloys: Mgâ€“Li system as test case. Intermetallics, 2012, 21, 88-96.	3.9	15
29	Evolving microstructure in MnO2 using amorphisation and recrystallisation. Journal of Crystal Growth, 2006, 294, 118-129.	1.5	13
30	Thermodynamic stability and pressure dependence of FePO4 polymorphs. Computational and Theoretical Chemistry, 2019, 1155, 67-74.	2.5	12
31	Atomistic Simulation and Characterization of Spinel Li_{1+x}Mn₂O₄ (0 â‰ x â‰ 1) Nanoparticles. ACS Applied Energy Materials, 2020, 3, 1429-1438.	5.1	12
32	Phase transformation and crystal structure of IrTi. Intermetallics, 2012, 31, 26-33.	3.9	11
33	Periodic modeling of zeolite Ti-LTA. Journal of Chemical Physics, 2017, 147, 074701.	3.0	11
34	Density Functional Theory Study of Ethylene Carbonate Adsorption on the (0001) Surface of Aluminum Oxide Î±-Al₂O₃. ACS Omega, 2021, 6, 29577-29587.	3.5	11
35	First-principles study: Effect of lithium and sodium intercalation in transition metal phosphates, MPO4 (M: Mn, Fe, Co). Computational Condensed Matter, 2020, 22, e00437.	2.1	10
36	Generating structural distributions of atomistic models of Li2O nanoparticles using simulated crystallisation. Journal of Materials Chemistry, 2010, 20, 10452.	6.7	8

#	Article	IF	Citations
37	The effects of process parameters on the properties of manganese-rich carbonate precursors: A study of co-precipitation synthesis using semi-batch reactors. Chemical Engineering Science, 2021, 241, 116694.	3.8	8
38	Structure of Surface Entrance Sites for Li Intercalation into TiO₂ Nanoparticles, Nanosheets, and Mesoporous Architectures with Application for Li-Ion Batteries. Journal of Physical Chemistry C, 2016, 120, 14001-14008.	3.1	6
39	Structural, thermodynamic, electronic and mechanical properties of spinel and phonon-harvested AMn2O4 (a: Li, Na, Mg) systems: A First-Principles study. Materials Today Communications, 2020, 22, 100704.	1.9	6
40	Brillouin scattering investigation of the rare-earth fluorides at high temperatures. Journal of the Less Common Metals, 1989, 148, 375-380.	0.8	5
41	â€˜Breathing-crystalsâ€™ the origin of electrochemical activity of mesoporous Liâ€“MnO₂. Journal of Materials Chemistry A, 2016, 4, 6456-6464.	10.3	5
42	First Principles Study of Oxygen Adsorption on Li-MO₂ (M = Mn, Ti and V) (110) Surface. Journal of the Electrochemical Society, 2021, 168, 070556.	2.9	5
43	Structural characterisation and mechanical properties of nanosized spinel LiMn2O4 cathode investigated using atomistic simulation. Materials Research Bulletin, 2022, 146, 111611.	5.2	5
44	Unravelling the Catalytic Activity of MnO₂, TiO₂, and VO₂ (110) Surfaces by Oxygen Coadsorption on Sodium-Adsorbed MO₂ {M = Mn, Ti, V}. ACS Omega, 0, , .	3.5	5
45	Brillouin scattering studies and computational simulations of the elastic properties of pyrite (FeS2) at high temperatures. Physica Status Solidi C: Current Topics in Solid State Physics, 2004, 1, 3073-3076.	0.8	4
46	Light scattering and computer simulation studies of superionic pure and La-doped BaF2. Chemical Physics, 2016, 467, 6-12.	1.9	2
47	Advances in Ti-Based Systems as High Temperature Shape Memory Alloys. Key Engineering Materials, 2018, 770, 230-238.	0.4	2
48	Discharge induced structural variation of simulated bulk Li1+xMn2O4 (0 â‰¤ x â‰¤ 1). Optical Materials, 2019, 92, 67-70.	3.6	2
49	Simulated synthesis and structure of LixTiO2 nanosheets as anode material for lithium ion batteries. Optical Materials, 2020, 102, 109831.	3.6	2
50	Phase stability of TiPd1-xRux and Ti1-xPdRux shape memory alloys. Materials Today: Proceedings, 2021, 38, 1071-1076.	1.8	2
51	Light scattering and computational simulations of the superionic behaviour of CaF2 doped with lanthanide ions. Physica Status Solidi C: Current Topics in Solid State Physics, 2005, 2, 490-494.	0.8	1
52	Computational Modelling as a Value Add in Energy Storage Materials. Nanostructure Science and Technology, 2016, , 481-513.	0.1	1
53	Oxidation behaviour of sperrylite and platarsite (100) surfaces: A DFT study. Materials Today Communications, 2022, 32, 103868.	1.9	1
54	Temperature Dependence and Martensitic Transformation of Ti₅₀Pt₅₀ Shape Memory Alloys. Advanced Materials Research, 0, 1019, 379-384.	0.3	0

#	Article	IF	Citations
55	Martensitic Transformation Behaviour of Ti₅₀Pt_{50-x}Co_x Shape Memory Alloys. Advanced Materials Research, 2014, 1019, 385-390.	0.3	0
56	First Principle Study of Ti₅₀Al₅₀ Alloys. Key Engineering Materials, 2018, 770, 224-229.	0.4	0
57	Synthesis of the porous spinel Co-Al2O4 powder produced by ball milling and annealing. Advanced Powder Technology, 2020, 31, 2742-2748.	4.1	0
58	Intercalation voltages for spinel LixMn2O4 (0â‰¤xâ‰¤2) cathode materials: Calibration of calculations with the ONETEP linear-scaling DFT code. Materials Today Communications, 2021, 27, 102380.	1.9	0