Sergiu Arapan

List of Publications by Year
in descending order

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Version: 2024-02-01

31	614	623574	580701
papers	citations	14 h-index	25 g-index

31	31	31	885
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	MAELAS 2.0: A new version of a computer program for the calculation of magneto-elastic properties. Computer Physics Communications, 2022, 271, 108197.	3.0	5
2	Spin-lattice model for cubic crystals. Physical Review B, 2021, 103, .	1.1	15
3	MAELAS: MAgneto-ELAStic properties calculation via computational high-throughput approach. Computer Physics Communications, 2021, 264, 107964.	3.0	10
4	Computational Design of Rare-Earth Reduced Permanent Magnets. Engineering, 2020, 6, 148-153.	3.2	22
5	MAELASviewer: An Online Tool to Visualize Magnetostriction. Sensors, 2020, 20, 6436.	2.1	4
6	Computational screening of Fe-Ta hard magnetic phases. Physical Review B, 2020, 101, .	1.1	11
7	Large scale and linear scaling DFT with the CONQUEST code. Journal of Chemical Physics, 2020, 152, 164112.	1.2	55
8	Database of novel magnetic materials for high-performance permanent magnet development. Computational Materials Science, 2019, 168, 188-202.	1.4	41
9	Influence of antiphase boundary of the MnAl Ï„ -phase on the energy product. Physical Review Materials, 2019, 3, .	0.9	1
10	A high-throughput exploration of magnetic materials by using structure predicting methods. Journal of Applied Physics, 2018, 123, .	1.1	9
11	Publisher's Note: Atomistic spin dynamics simulations of the MnAl <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mi>Ï„</mml:mi></mml:math> -phase and its antiphase boundary [Phys. Rev. B 96 , 224411 (2017)]. Physical Review B, 2018, 97, .	1.1	0
12	Exploring the Crystal Structure Space of CoFe₂P by Using Adaptive Genetic Algorithm Methods. IEEE Transactions on Magnetics, 2017, 53, 1-5.	1.2	3
13	Atomistic spin dynamics simulations of the MnAl <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mi>Ï„</mml:mi></mml:math> -phase and its antiphase boundary. Physical Review B, 2017, 96, .	1.1	18
14	Applying highâ€throughput computational techniques for discovering nextâ€generation of permanent magnets. Physica Status Solidi C: Current Topics in Solid State Physics, 2016, 13, 942-950.	0.8	4
15	Volume-dependent electron localization in ceria. Physical Review B, 2015, 91, .	1.1	16
16	Large-scale DFT simulations with a linear-scaling DFT code CONQUEST on K-computer. Journal of Advanced Simulation in Science and Engineering, 2014, 1, 87-97.	0.1	22
17	Information-Theoretic Approach for the Discovery of Design Rules for Crystal Chemistry. Journal of Chemical Information and Modeling, 2012, 52, 1812-1820.	2.5	40
18	Temperature-driven Î±-to-Î² phase transformation in Ti, Zr and Hf from first-principles theory combined with lattice dynamics. Europhysics Letters, 2011, 96, 66006.	0.7	27

#	Article	IF	Citations
19	Anab initiomolecular dynamics study of iron phases at high pressure and temperature. Journal of Physics Condensed Matter, 2011, 23, 485402.	0.7	19
20	Dynamical stability of body center cubic iron at the Earthâ€™s core conditions. Proceedings of the National Academy of Sciences of the United States of America, 2010, 107, 9962-9964.	3.3	58
21	High-pressure phase transformations in carbonates. Physical Review B, 2010, 82, .	1.1	31
22	MgO phase diagram from first principles in a wide pressure-temperature range. Physical Review B, 2010, 81, .	1.1	85
23	Determination of the Structural Parameters of an Incommensurate Phase from First Principles: The Case of Sc-II. Physical Review Letters, 2009, 102, 085701.	2.9	15
24	Prediction of incommensurate crystal structure in Ca at high pressure. Proceedings of the National Academy of Sciences of the United States of America, 2008, 105, 20627-20630.	3.3	45
25	Electronic structure of Cu3N films studied by soft x-ray spectroscopy. Journal of Physics Condensed Matter, 2008, 20, 235212.	0.7	12
26	High-pressure phase transformations in aragonite, strontianite and witherite. Acta Crystallographica Section A: Foundations and Advances, 2008, 64, C205-C205.	0.3	0
27	Formation ofsp3Hybridized Bonds and Stability ofCaCO3at Very High Pressure. Physical Review Letters, 2007, 98, 268501.	2.9	32
28	Exciton levels and optical absorption in coupled double quantum well structures. Journal of Luminescence, 2005, 112, 216-219.	1.5	9
29	Conductance of a disordered double quantum wire in a magnetic field: Boundary roughness scattering. Physical Review B, 2003, 67, .	1.1	5
30	Effect of the boundary roughness on the conductance of double quantum wire in a magnetic field. Europhysics Letters, 2003, 64, 239-245.	0.7	0
31	Spin-orbit interaction and spintronics effects in semiconductor structures driven by interband coupling through optical phonon like displacements. , 0, , .		0