

Aleksei V Ivanov

List of Publications by Year in descending order

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Version: 2024-02-01

15
papers

177
citations

1162889

8
h-index

1058333

14
g-index

15
all docs

15
docs citations

15
times ranked

148
citing authors

#	ARTICLE	IF	CITATIONS
1	Variational Density Functional Calculations of Excited States: Conical Intersection and Avoided Crossing in Ethylene Bond Twisting. <i>Journal of Physical Chemistry Letters</i> , 2022, 13, 3990-3999.	2.1	9
2	Fast and robust algorithm for energy minimization of spin systems applied in an analysis of high temperature spin configurations in terms of skyrmion density. <i>Computer Physics Communications</i> , 2021, 260, 107749.	3.0	13
3	Mn Dimer Can Be Described Accurately with Density Functional Calculations When Self-Interaction Correction Is Applied. <i>Journal of Physical Chemistry Letters</i> , 2021, 12, 4240-4246.	2.1	7
4	Method for Calculating Excited Electronic States Using Density Functionals and Direct Orbital Optimization with Real Space Grid or Plane-Wave Basis Set. <i>Journal of Chemical Theory and Computation</i> , 2021, 17, 5034-5049.	2.3	12
5	Assessment of the Accuracy of Density Functionals for Calculating Oxygen Reduction Reaction on Nitrogen-Doped Graphene. <i>Journal of Chemical Theory and Computation</i> , 2021, 17, 6405-6415.	2.3	9
6	Direct energy minimization based on exponential transformation in density functional calculations of finite and extended systems. <i>Computer Physics Communications</i> , 2021, 267, 108047.	3.0	7
7	Chemical bonding theories as guides for self-interaction corrected solutions: Multiple local minima and symmetry breaking. <i>Journal of Chemical Physics</i> , 2021, 155, 224109.	1.2	7
8	Variational Density Functional Calculations of Excited States via Direct Optimization. <i>Journal of Chemical Theory and Computation</i> , 2020, 16, 6968-6982.	2.3	45
9	Efficient optimization method for finding minimum energy paths of magnetic transitions. <i>Journal of Physics Condensed Matter</i> , 2020, 32, 345901.	0.7	12
10	Variational calculations of excited states via direct optimization of the orbitals in DFT. <i>Faraday Discussions</i> , 2020, 224, 448-466.	1.6	31
11	Fully self-consistent calculations of magnetic structure within non-collinear Alexander-Anderson model. <i>Nanosystems: Physics, Chemistry, Mathematics</i> , 2020, 11, 65-77.	0.2	2
12	Multiple minimum-energy paths and scenarios of unwinding transitions in chiral nematic liquid crystals. <i>Physical Review E</i> , 2019, 100, 062704.	0.8	5
13	Magnetic exchange force microscopy: theoretical analysis of induced magnetization reversals. <i>Nanoscale</i> , 2017, 9, 13320-13325.	2.8	12
14	Tip-surface interaction and rate of magnetic transitions. <i>Journal of Physics: Conference Series</i> , 2016, 741, 012184.	0.3	0
15	Energy surface and minimum energy paths for Fréedericksz transitions in bistable cholesteric liquid crystals. <i>Physical Review E</i> , 2016, 93, 042708.	0.8	6