

Aleksei V Ivanov

List of Publications by Year in descending order

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#	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.	4.6	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.	7.5	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.	4.6	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.	5.3	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.	5.3	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.	7.5	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.	3.0	7
8	Variational Density Functional Calculations of Excited States via Direct Optimization. <i>Journal of Chemical Theory and Computation</i> , 2020, 16, 6968-6982.	5.3	45
9	Efficient optimization method for finding minimum energy paths of magnetic transitions. <i>Journal of Physics Condensed Matter</i> , 2020, 32, 345901.	1.8	12
10	Variational calculations of excited states via direct optimization of the orbitals in DFT. <i>Faraday Discussions</i> , 2020, 224, 448-466.	3.2	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.	0.4	2
12	Multiple minimum-energy paths and scenarios of unwinding transitions in chiral nematic liquid crystals. <i>Physical Review E</i> , 2019, 100, 062704.	2.1	5
13	Magnetic exchange force microscopy: theoretical analysis of induced magnetization reversals. <i>Nanoscale</i> , 2017, 9, 13320-13325.	5.6	12
14	Tip-surface interaction and rate of magnetic transitions. <i>Journal of Physics: Conference Series</i> , 2016, 741, 012184.	0.4	0
15	Energy surface and minimum energy paths for Fréedericksz transitions in bistable cholesteric liquid crystals. <i>Physical Review E</i> , 2016, 93, 042708.	2.1	6