Sijie Luo

List of Publications by Year
in descending order

11	907	1039880 9	1199470 12
papers	citations	h-index	g-index

12	12	12	1386
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Multiconfiguration Pair-Density Functional Theory. Journal of Chemical Theory and Computation, 2014, 10, 3669-3680.	2.3	334
2	Bulk Properties of Transition Metals: A Challenge for the Design of Universal Density Functionals. Journal of Chemical Theory and Computation, 2014, 10, 3832-3839.	2.3	245
3	Validation of electronic structure methods for isomerization reactions of large organic molecules. Physical Chemistry Chemical Physics, 2011, 13, 13683.	1.3	78
4	Density Functional Theory of Open-Shell Systems. The 3d-Series Transition-Metal Atoms and Their Cations. Journal of Chemical Theory and Computation, 2014, 10, 102-121.	2.3	65
5	Improved CO Adsorption Energies, Site Preferences, and Surface Formation Energies from a Meta-Generalized Gradient Approximation Exchangeâ€“Correlation Functional, M06-L. Journal of Physical Chemistry Letters, 2012, 3, 2975-2979.	2.1	63
6	How Evenly Can Approximate Density Functionals Treat the Different Multiplicities and Ionization States of 4d Transition Metal Atoms?. Journal of Chemical Theory and Computation, 2012, 8, 4112-4126.	2.3	37
7	Noncollinear Spins Provide a Self-Consistent Treatment of the Low-Spin State of a Biomimetic Oxomanganese Synthetic Trimer Inspired by the Oxygen Evolving Complex of Photosystem II. Journal of Physical Chemistry Letters, 2011, 2, 2629-2633.	2.1	29
8	The Structure of Silica Surfaces Exposed to Atomic Oxygen. Journal of Physical Chemistry C, 2013, 117, 9311-9321.	1.5	28
9	Noncollinear Spin States for Density Functional Calculations of Open-Shell and Multi-Configurational Systems: Dissociation of MnO and NiO and Barrier Heights of O₃, BeH₂, and H₄. Journal of Chemical Theory and Computation, 2013, 9, 5349-5355.	2.3	14
10	Computational Electrochemistry. Voltages of Lithium-Ion Battery Cathodes. Journal of Physical Chemistry B, 2016, 120, 1437-1439.	1.2	6
11	Ligand-Mediated Ring â†' Cube Transformation in a Catalytic Subnanocluster: Co₄O₄(MeCN)_n with n = 1â€“6. Journal of Physical Chemistry Letters, 2014, 5, 2528-2532.	2.1	5