Sijie Luo

List of Publications by Year in Descending Order

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The third column is the impact factor (IF) of the journal, and the fourth column is the number of citations of the article.

11 papers	724 citations	9 h-index	12 g-index
12 ext. papers	821 ext. citations	5.5 avg, IF	3.81 L-index

#	Paper	IF	Citations
11	Computational Electrochemistry. Voltages of Lithium-Ion Battery Cathodes. *Journal of Physical Chemistry B*, **2016**, 120, 1437-9	3.4	5
10	Density Functional Theory of Open-Shell Systems. The 3d-Series Transition-Metal Atoms and Their Cations. *Journal of Chemical Theory and Computation*, **2014**, 10, 102-21	6.4	55
9	Multiconfiguration Pair-Density Functional Theory. *Journal of Chemical Theory and Computation*, **2014**, 10, 3669-80	6.4	246
8	Ligand-Mediated Ring -zCube Transformation in a Catalytic Subnanocluster: Co4O4(MeCN)n with n = 1-6. *Journal of Physical Chemistry Letters*, **2014**, 5, 2528-32	6.4	5
7	Bulk Properties of Transition Metals: A Challenge for the Design of Universal Density Functionals. *Journal of Chemical Theory and Computation*, **2014**, 10, 3832-9	6.4	187
6	The Structure of Silica Surfaces Exposed to Atomic Oxygen. *Journal of Physical Chemistry C*, **2013**, 117, 9311-9321	3.8	22
5	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, 5349-55	6.4	13
4	Improved CO Adsorption Energies, Site Preferences, and Surface Formation Energies from a Meta-Generalized Gradient Approximation Exchange-Correlation Functional, M06-L. *Journal of Physical Chemistry Letters*, **2012**, 3, 2975-9	6.4	59
3	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, 4112-26	6.4	34
2	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	6.4	28
1	Validation of electronic structure methods for isomerization reactions of large organic molecules. *Physical Chemistry Chemical Physics*, **2011**, 13, 13683-9	3.6	67