Jorge Aguilera-Iparraguirre

List of Publications by Year
in descending order

13 papers	3,173 citations	933447 10 h-index	1125743 13 g-index
13 all docs	13 docs citations	13 times ranked	4000 citing authors

#	Article	IF	Citations
1	Automatic Chemical Design Using a Data-Driven Continuous Representation of Molecules. ACS Central Science, 2018, 4, 268-276.	11.3	1,761
2	An Alternative Host Material for Longâ€Lifespan Blue Organic Lightâ€Emitting Diodes Using Thermally Activated Delayed Fluorescence. Advanced Science, 2017, 4, 1600502.	11.2	103
3	Turbocharged molecular discovery of OLED emitters: from high-throughput quantum simulation to highly efficient TADF devices. Proceedings of SPIE, 2016, , .	0.8	3
4	Design of efficient molecular organic light-emitting diodes by a high-throughput virtual screening and experimental approach. Nature Materials, 2016, 15, 1120-1127.	27.5	708
5	34.4: Invited Paper: Combinatorial Design of OLEDâ€Emitting Materials. Digest of Technical Papers SID International Symposium, 2015, 46, 505-506.	0.3	3
6	What Is High-Throughput Virtual Screening? A Perspective from Organic Materials Discovery. Annual Review of Materials Research, 2015, 45, 195-216.	9.3	203
7	A kinetic and thermochemical database for organic sulfur and oxygen compounds. Physical Chemistry Chemical Physics, 2015, 17, 13625-13639.	2.8	16
8	New Pathways for Formation of Acids and Carbonyl Products in Low-Temperature Oxidation: The Korcek Decomposition of Î³-Ketohydroperoxides. Journal of the American Chemical Society, 2013, 135, 11100-11114.	13.7	153
9	Detailed chemical kinetic modeling of JPâ€10 (exoâ€tetrahydrodicyclopentadiene) highâ€temperature oxidation: Exploring the role of biradical species in initial decomposition steps. International Journal of Chemical Kinetics, 2012, 44, 179-193.	1.6	43
10	Accurate Coupled Cluster Calculations of the Reaction Barrier Heights of Two CH₃^{â€¢} + CH₄ Reactions. Journal of Physical Chemistry A, 2009, 113, 11679-11684.	2.5	10
11	Accurate ab initio computation of thermochemical data for C3Hx species. Chemical Physics, 2008, 346, 56-68.	1.9	37
12	Accurate Benchmark Calculation of the Reaction Barrier Height for Hydrogen Abstraction by the Hydroperoxyl Radical from Methane. Implications for C_nH_{2n+2} where n = 2 â† 4. Journal of Physical Chemistry A, 2008, 112, 7047-7054.	2.5	105
13	Density Functional Theory Study of the Formation of Naphthalene and Phenanthrene from Reactions of Phenyl with Vinyl- and Phenylacetylene. Journal of Chemical Theory and Computation, 2007, 3, 139-145.	5.3	28