William Paul Huhn

List of Publications by Year
in descending order

17 papers	1,077 citations	567144 15 h-index	887953 17 g-index
18 all docs	18 docs citations	18 times ranked	1798 citing authors

#	Article	IF	Citations
1	The CECAM electronic structure library and the modular software development paradigm. Journal of Chemical Physics, 2020, 153, 024117.	1.2	19
2	ELSI â€" An open infrastructure for electronic structure solvers. Computer Physics Communications, 2020, 256, 107459.	3.0	27
3	GPU acceleration of all-electron electronic structure theory using localized numeric atom-centered basis functions. Computer Physics Communications, 2020, 254, 107314.	3.0	30
4	ELSI: A unified software interface for Kohnâ€"Sham electronic structure solvers. Computer Physics Communications, 2018, 222, 267-285.	3.0	78
5	Tunable Semiconductors: Control over Carrier States and Excitations in Layered Hybrid Organic-Inorganic Perovskites. Physical Review Letters, 2018, 121, 146401.	2.9	103
6	Band Gap Tailoring and Structure-Composition Relationship within the Alloyed Semiconductor Cu₂BaGe_{1â€"x}Sn_xSe₄. Chemistry of Materials, 2018, 30, 6566-6574.	3.2	25
7	Thermodynamic Equilibria in Carbon Nitride Photocatalyst Materials and Conditions for the Existence of Graphitic Carbon Nitride g-C₃N₄. Chemistry of Materials, 2017, 29, 4445-4453.	3.2	58
8	The Elephant in the Room of Density Functional Theory Calculations. Journal of Physical Chemistry Letters, 2017, 8, 1449-1457.	2.1	88
9	I₂â€"IIâ€"IVâ€"VI₄ (I = Cu, Ag; II = Sr, Ba; IV = Ge, Sn; VI = S, Se): Chalcogenides for Thin-Film Photovoltaics. Chemistry of Materials, 2017, 29, 7868-7879.	3.2	87
10	Candidate photoferroic absorber materials for thin-film solar cells from naturally occurring minerals: enargite, stephanite, and bournonite. Sustainable Energy and Fuels, 2017, 1, 1339-1350.	2.5	32
11	One-hundred-three compound band-structure benchmark of post-self-consistent spin-orbit coupling treatments in density functional theory. Physical Review Materials, 2017, 1, .	0.9	92
12	Direct and cost-efficient hyperpolarization of long-lived nuclear spin states on universal ¹⁵ N ₂ -diazirine molecular tags. Science Advances, 2016, 2, e1501438.	4.7	193
13	BaCu₂Sn(S,Se)₄: Earth-Abundant Chalcogenides for Thin-Film Photovoltaics. Chemistry of Materials, 2016, 28, 4771-4780.	3.2	131
14	First-principles calculation of elastic moduli of early-late transition metal alloys. Physical Review B, 2014, 89, .	1.1	8
15	First principles modeling of the temperature dependent ternary phase diagram for the Cuâ€"Pdâ€"S system. Computational Materials Science, 2014, 92, 377-386.	1.4	1
16	A Free Energy Model of Boron Carbide. Journal of Statistical Physics, 2013, 150, 432-441.	0.5	18
17	Prediction of A2 to B2 Phase Transition in the High-Entropy Alloy Mo-Nb-Ta-W. Jom, 2013, 65, 1772-1779.	0.9	87