

List of Publications by Year in descending order

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#	Article	IF	CITATIONS
1	New schemes for internally contracted multi-reference configuration interaction. Journal of Chemical Physics, 2014, 141, 164114.	3.0	19
2	Modulating the magnetic properties of MoS ₂ monolayers by group VIII doping and vacancy engineering. RSC Advances, 2018, 8, 18837-18850.	3.6	15
3	Highly Selective Electrocatalytic CO ₂ Reduction to Methanol on Iridium Dioxide with CO [*] Spectators. ChemElectroChem, 2020, 7, 5036-5043.	3.4	9
4	From orientation disordered to ordered-Anab initiosimulation on ammonia borane phase transition within van der Waals corrections. Journal of Computational Chemistry, 2015, 36, 22-32.	3.3	4
5	Doping Kinetics and Structural Studies for Lithiumâ€rich Mnâ€based Lithium Ion Cathode Materials. Energy Technology, 2021, 9, 2000894.	3.8	4
6	A first-principles simulation of the metal borohydride ammonia borane complex (LiBH4)2(NH3BH3) and the decomposition reaction pathway for hydrogen storage. International Journal of Hydrogen Energy, 2019, 44, 20121-20132.	7.1	3
7	A theoretical study on the role of ammonium ions in the double-layered V ₂ O ₅ electrode. Physical Chemistry Chemical Physics, 2021, 23, 4187-4194.	2.8	3
8	A theoretical explanation of RbBH4's fractionally occupied ground-state phase and the reorientational motion of the [BH4]â^' group. Journal Physics D: Applied Physics, 2017, 50, 455501.	2.8	3
9	First-principles study of the reorientational motion of the [BH4]- groups in CsBH4's fractionally occupied ground-state phase and the thermal properties. Physica B: Condensed Matter, 2019, 564, 69-79.	2.7	1
10	Origin of the structural diversity of the alkaline metal borohydride MBH4 (MÂ=ÂLi, Na, K, Rb and Cs): Insights from first-principles calculations. International Journal of Hydrogen Energy, 2020, 45, 9946-9958.	7.1	1