Katarina BataloviÄ

List of Publications by Year
in descending order

22 papers	398 citations	759055 12 h-index	752573 20 g-index
23 all docs	23 docs citations	23 times ranked	623 citing authors

#	Article	IF	Citations
1	DFT study of crystal structure and electronic properties of metal-doped AlH3 polymorphs. International Journal of Hydrogen Energy, 2022, 47, 6142-6153.	3.8	6
2	Predicting the Heat of Hydride Formation by Graph Neural Network â€•Exploring the Structureâ€“Property Relation for Metal Hydrides. Advanced Theory and Simulations, 2022, 5, .	1.3	6
3	Mechanochemical modification of LiAlH4 with Fe2O3 - A combined DFT and experimental study. International Journal of Hydrogen Energy, 2021, 46, 13070-13081.	3.8	7
4	Origin of photocatalytic activity enhancement in Pd/Pt-deposited anatase N-TiO₂ â€“ experimental insights and DFT study of the (001) surface. Physical Chemistry Chemical Physics, 2020, 22, 18536-18547.	1.3	6
5	Influence of Defects on the Stability and Hydrogenâ€Sorption Behavior of Mgâ€Based Hydrides. ChemPhysChem, 2019, 20, 1216-1247.	1.0	22
6	Modification of N-doped TiO₂ photocatalysts using noble metals (Pt, Pd) â€“ a combined XPS and DFT study. Physical Chemistry Chemical Physics, 2017, 19, 7062-7071.	1.3	60
7	Study on electronic properties of Î±-, Î²- and Î³-AlH 3 â€“ The theoretical approach. Computational Materials Science, 2017, 134, 100-108.	1.4	8
8	Theoretical investigation of interaction of hydrogen and intermetallic compound YCo5. Journal of Alloys and Compounds, 2017, 726, 1085-1091.	2.8	0
9	BiFeO3 perovskites: A multidisciplinary approach to multiferroics. Ceramics International, 2017, 43, 1256-1264.	2.3	73
10	Effect of PEO molecular weight on sunlight induced photocatalytic activity of ZnO/PEO composites. Solar Energy, 2016, 127, 124-135.	2.9	13
11	Enhancing photocatalytic properties of rutile TiO2 by codoping with N and metals â€“ Ab initio study. International Journal of Hydrogen Energy, 2015, 40, 9696-9703.	3.8	17
12	Hydrogen diffusion in MgH₂ doped with Ti, Mn andÂFe. RSC Advances, 2015, 5, 34894-34899.	1.7	25
13	Influence of Ta and Nb on the hydrogen absorption kinetics in Zr-based alloys. International Journal of Hydrogen Energy, 2015, 40, 5677-5682.	3.8	14
14	Density functional theory guide to structure and thermodynamics of metal hydrides â€“ Case study of (Ti, Zr, Hf)Ni intermetallic compounds. International Journal of Hydrogen Energy, 2015, 40, 13029-13038.	3.8	9
15	Interstitial hydrogen in Laves phases â€“ local electronic structure modifications from first-principles. RSC Advances, 2014, 4, 54769-54774.	1.7	6
16	Transition metal doping of Mg₂FeH₆â€“ a DFT insight into synthesis and electronic structure. Physical Chemistry Chemical Physics, 2014, 16, 12356-12361.	1.3	20
17	Hydrogen Storage in Martensite Tiâ€“Zrâ€“Ni Alloy: A Density Functional Theory Study. Journal of Physical Chemistry C, 2013, 117, 26914-26920.	1.5	13
18	Kinetics of hydrogen absorption in Zr-based alloys. Journal of Alloys and Compounds, 2013, 559, 162-166.	2.8	14

#	Article	IF	Citations
19	A study on crystal structure, bonding and hydriding properties of Tiâ€“Feâ€“Ni intermetallics â€“ Behind substitution of iron by nickel. International Journal of Hydrogen Energy, 2012, 37, 8408-8417.	3.8	48
20	Hydrogenation properties of Hfâ€“Ni intermetallics â€“ Experimental and theoretical investigation. International Journal of Hydrogen Energy, 2011, 36, 10771-10778.	3.8	6
21	HfNi and its hydrides â€“ First principles calculations. International Journal of Hydrogen Energy, 2010, 35, 3572-3577.	3.8	17
22	First-principles study of the thermodynamic properties and electronic structure of compounds from Hfâ€“Ni phase system. Computational Materials Science, 2010, 49, 55-59.	1.4	8