Barbara Szpunar

List of Publications by Year
in descending order

15	206	1040056 9	1199594 12
papers	citations	h-index	g-index

17	17	17	199
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	First-principles investigation of electronsâ€™ thermal excitations in UN, UAl2 and ThN. Solid State Communications, 2021, 323, 114131.	1.9	0
2	First principles investigation of thermal properties of thorium mononitride. Journal of Alloys and Compounds, 2021, 879, 160467.	5.5	6
3	Density Functional Theory Study of Oxygen Adsorption and Dissociation on Lower Miller Index Surfaces of ThN. Journal of Physical Chemistry C, 2020, 124, 24849-24860.	3.1	7
4	First principles investigation of thermal transport of uranium mononitride. Journal of Physics and Chemistry of Solids, 2020, 146, 109636.	4.0	21
5	DFT +UStudy of the Adsorption and Dissociation of Water on Clean, Defective, and Oxygen-Covered U₃Si₂{001}, {110}, and {111} Surfaces. Journal of Physical Chemistry C, 2019, 123, 19453-19467.	3.1	13
6	Thermal conductivity of bulk and porous ThO2: Atomistic and experimental study. Journal of Alloys and Compounds, 2019, 798, 507-516.	5.5	26
7	Atomistic and experimental study on thermal conductivity of bulk and porous cerium dioxide. Scientific Reports, 2019, 9, 6326.	3.3	20
8	Atomistic modeling of thermoâ€mechanical properties of cubic SiC. Journal of the American Ceramic Society, 2018, 101, 4753-4762.	3.8	13
9	Thermal conductivity of bulk and nanowire of cubic-SiC from ab initio calculations. Computational Materials Science, 2017, 128, 249-256.	3.0	24
10	Firstâ€Principles Molecular Dynamics Studies of Oxygen Sublattice Melting in Thoria. Journal of the American Ceramic Society, 2016, 99, 1494-1497.	3.8	0
11	First principles calculation of thermo-mechanical properties of thoria using Quantum ESPRESSO. International Journal of Computational Materials Science and Engineering, 2016, 05, 1650008.	0.7	8
12	An Interface to Quantum ESPRESSO. , 2015, , 155-162.		8
13	Molecular Dynamics Study of Hydrogen in Î±-Zirconium. International Journal of Nuclear Energy, 2014, 2014, 1-6.	0.4	9
14	Density functional studies of selected metal dioxides. Journal of Physics and Chemistry of Solids, 2013, 74, 1632-1639.	4.0	15
15	Thermal expansion and hydrogen diffusion in nanocrystalline nickel. Physical Review B, 1999, 60, 10107-10113.	3.2	30