

# Barbara Szpunar

## List of Publications by Year in descending order

Source: <https://exaly.com/author-pdf/4466932/publications.pdf>

Version: 2024-02-01

15

papers

206

citations

1040056

9

h-index

1199594

12

g-index

17

all docs

17

docs citations

17

times ranked

199

citing authors

#	ARTICLE	IF	CITATIONS
1	Thermal expansion and hydrogen diffusion in nanocrystalline nickel. Physical Review B, 1999, 60, 10107-10113.	3.2	30
2	Thermal conductivity of bulk and porous ThO <sub>2</sub> : Atomistic and experimental study. Journal of Alloys and Compounds, 2019, 798, 507-516.	5.5	26
3	Thermal conductivity of bulk and nanowire of cubic-SiC from ab initio calculations. Computational Materials Science, 2017, 128, 249-256.	3.0	24
4	First principles investigation of thermal transport of uranium mononitride. Journal of Physics and Chemistry of Solids, 2020, 146, 109636.	4.0	21
5	Atomistic and experimental study on thermal conductivity of bulk and porous cerium dioxide. Scientific Reports, 2019, 9, 6326.	3.3	20
6	Density functional studies of selected metal dioxides. Journal of Physics and Chemistry of Solids, 2013, 74, 1632-1639.	4.0	15
7	Atomistic modeling of thermo-mechanical properties of cubic SiC. Journal of the American Ceramic Society, 2018, 101, 4753-4762.	3.8	13
8	DFT + <i>i</i> U Study of the Adsorption and Dissociation of Water on Clean, Defective, and Oxygen-Covered $\text{Si}_{3}\text{Si}_{2}$ {001}, {110}, and {111} Surfaces. Journal of Physical Chemistry C, 2019, 123, 19453-19467.	3.1	13
9	Molecular Dynamics Study of Hydrogen in $\text{Zr}_{1-x}\text{H}_x$ -Zirconium. International Journal of Nuclear Energy, 2014, 2014, 1-6.	0.4	9
10	An Interface to Quantum ESPRESSO. , 2015, , 155-162.		8
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	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
13	First principles investigation of thermal properties of thorium mononitride. Journal of Alloys and Compounds, 2021, 879, 160467.	5.5	6
14	First-principles Molecular Dynamics Studies of Oxygen Sublattice Melting in Thoria. Journal of the American Ceramic Society, 2016, 99, 1494-1497.	3.8	0
15	First-principles investigation of electrons' thermal excitations in UN, UAl <sub>2</sub> and ThN. Solid State Communications, 2021, 323, 114131.	1.9	0