GÃ¶ran WahnstrÃ¶m

List of Publications by Year
in descending order

39 papers	1,388 citations	304743 22 h-index	330143 37 g-index
39 all docs	39 docs citations	39 times ranked	1391 citing authors

#	Article	IF	Citations
1	Thermodynamics of doping and vacancy formation inBaZrO3perovskite oxide from density functional calculations. Physical Review B, 2006, 73, .	3.2	139
2	Structure and thermodynamic stability of hydrogen interstitials in BaZrO3perovskite oxide from density functional calculations. Faraday Discussions, 2007, 134, 247-265.	3.2	116
3	Density-functional calculations of prefactors and activation energies for H diffusion in<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:mi mathvariant="normal">Ba</mml:mi><mml:mi mathvariant="normal">Zr</mml:mi><mml:msub><mml:mi mathvariant="normal">O</mml:mi><mml:mn>3</mml:mn></mml:msub></mml:mrow></mml:math>. Physical Review B, 2007, 76, .	3.2	98
4	Motion of â€˜â€˜hotâ€™â€™ oxygen adatoms on corrugated metal surfaces. Journal of Chemical Physics, 1996, 105, 326-336.	3.0	85
5	Motion of nanometer sized magnetic particles in a magnetic field gradient. Journal of Applied Physics, 2008, 104, .	2.5	72
6	Effect of Boron on Carbide Coarsening at 873ÂK (600ÂÂ°C) in 9Âto 12Âpct Chromium Steels. Metallurgical and Materials Transactions A: Physical Metallurgy and Materials Science, 2012, 43, 4053-4062.	2.2	60
7	Size and shape of oxygen vacancies and protons in acceptor-doped barium zirconate. Solid State Ionics, 2015, 275, 2-8.	2.7	60
8	Oxygen vacancy segregation and space-charge effects in grain boundaries of dry and hydrated BaZrO3. Applied Physics Letters, 2012, 100, .	3.3	52
9	Effective magnetic moment of magnetic multicore nanoparticles. Physical Review B, 2009, 80, .	3.2	50
10	Quantitative Analysis of WC Grain Shape in Sintered WC-Co Cemented Carbides. Physical Review Letters, 2005, 94, 066105.	7.8	48
11	Path Integral Treatment of Proton Transport Processes inBaZrO3. Physical Review Letters, 2008, 101, 215902.	7.8	45
12	Transition Metal Solubilities in WC in Cemented Carbide Materials. Journal of the American Ceramic Society, 2011, 94, 605-610.	3.8	45
13	Using Neutron Spinâ^'Echo To Investigate Proton Dynamics in Proton-Conducting Perovskites. Chemistry of Materials, 2010, 22, 740-742.	6.7	43
14	Unraveling the Ground-State Structure of BaZrO₃ by Neutron Scattering Experiments and First-Principles Calculations. Chemistry of Materials, 2020, 32, 2824-2835.	6.7	41
15	Comparison of Space-Charge Formation at Grain Boundaries in Proton-Conducting BaZrO₃ and BaCeO₃. Chemistry of Materials, 2017, 29, 7931-7941.	6.7	39
16	Implications of the band gap problem on oxidation and hydration in acceptor-doped barium zirconate. Physical Review B, 2015, 91, .	3.2	36
17	Polaronic contributions to oxidation and hole conductivity in acceptor-doped<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mi>BaZrO</mml:mi><mml:mn>3</mml:mn></mml:msub></mml:math>. Physical Review B, 2016, 94, .	3.2	36
18	Defect segregation to grain boundaries in BaZrO₃ from first-principles free energy calculations. Journal of Materials Chemistry A, 2017, 5, 13421-13429.	10.3	30

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19	Oxygen vacancy segregation in grain boundaries of BaZrO3 using interatomic potentials. Solid State Ionics, 2013, 230, 27-31.	2.7	28
20	A computational study of interfaces in WCâ€“Co cemented carbides. Modelling and Simulation in Materials Science and Engineering, 2015, 23, 045001.	2.0	26
21	Local structure and vibrational dynamics in indium-doped barium zirconate. Journal of Materials Chemistry A, 2019, 7, 7360-7372.	10.3	24
22	Theory of ultrathin films at metalâ€“ceramic interfaces. Philosophical Magazine Letters, 2010, 90, 599-609.	1.2	23
23	Band vs. polaron: vibrational motion and chemical expansion of hydride ions as signatures for the electronic character in oxyhydride barium titanate. Journal of Materials Chemistry A, 2019, 7, 16211-16221.	10.3	22
24	Complexions and grain growth retardation: First-principles modeling of phase boundaries in WC-Co cemented carbides at elevated temperatures. Acta Materialia, 2021, 216, 117128.	7.9	22
25	A computational study of special grain boundaries in WCâ€“Co cemented carbides. Computational Materials Science, 2015, 98, 345-353.	3.0	19
26	First-principles investigation of the stability of MN and CrMN precipitates under coherency strains in Î±-Fe (Mâ€‰=â€‰V, Nb, Ta). Journal of Applied Physics, 2011, 109, .	2.5	17
27	<scp>dynasor</scp>â€”A Tool for Extracting Dynamical Structure Factors and Current Correlation Functions from Molecular Dynamics Simulations. Advanced Theory and Simulations, 2021, 4, 2000240.	2.8	15
28	High resolution STEM investigation of interface layers in cemented carbides. International Journal of Refractory Metals and Hard Materials, 2018, 72, 135-140.	3.8	14
29	Finite element simulations of thermal residual stresses in realistic 3D WC-Co microstructures. International Journal of Refractory Metals and Hard Materials, 2019, 85, 105065.	3.8	14
30	<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mi>BaZrO</mml:mi><mml:mn>3</mml:mn></mml:msub></m stability under pressure: The role of nonlocal exchange and correlation. Physical Review B, 2020, 101, .	3.2	12
31	Modeling of vibrational and configurational degrees of freedom in hexagonal and cubic tungsten carbide at high temperatures. Physical Review Materials, 2021, 5, .	2.4	10
32	The role of oxygen vacancies on the vibrational motions of hydride ions in the oxyhydride of barium titanate. Journal of Materials Chemistry A, 2020, 8, 6360-6371.	10.3	9
33	A computational study of the temperature dependence of interface and surface energies in WCâ€“Co cemented carbides. International Journal of Refractory Metals and Hard Materials, 2020, 87, 105114.	3.8	8
34	Low-frequency vibrations in monomers, dimers and polymers of propylene glycol. The Philosophical Magazine: Physics of Condensed Matter B, Statistical Mechanics, Electronic, Optical and Magnetic Properties, 1998, 77, 699-707.	0.6	7
35	Early stages of phase separation using three-dimensional atom probe and atomistic modelling. Surface and Interface Analysis, 2007, 39, 178-183.	1.8	7
36	CCBuilder: a software that produces synthetic microstructures of WC-Co cemented carbides. International Journal of Refractory Metals and Hard Materials, 2019, 78, 210-218.	3.8	7

#	Article	IF	Citations
37	Percolation Transition in Hole-Conducting Acceptor-Doped Barium Zirconate. Chemistry of Materials, 2020, 32, 5558-5568.	6.7	5
38	First-principles modeling of complexions at the phase boundaries in Ti-doped WC-Co cemented carbides at finite temperatures. Physical Review Materials, 2021, 5, .	2.4	4
39	H Motion in Pd and Nb: A Molecular-Dynamics Study. Materials Research Society Symposia Proceedings, 1992, 291, 537.	0.1	0