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	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
2	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
3	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
4	<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
5	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
6	Percolation Transition in Hole-Conducting Acceptor-Doped Barium Zirconate. Chemistry of Materials, 2020, 32, 5558-5568.	6.7	5
7	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
8	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
9	<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
10	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
11	Local structure and vibrational dynamics in indium-doped barium zirconate. Journal of Materials Chemistry A, 2019, 7, 7360-7372.	10.3	24
12	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
13	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
14	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
15	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
16	Comparison of Space-Charge Formation at Grain Boundaries in Proton-Conducting BaZrO₃ and BaCeO₃. Chemistry of Materials, 2017, 29, 7931-7941.	6.7	39
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></m Physical Review B, 2016, 94, .	3.2	36
18	Implications of the band gap problem on oxidation and hydration in acceptor-doped barium zirconate. Physical Review B, 2015, 91, .	3.2	36

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19	A computational study of interfaces in WCâ€“Co cemented carbides. Modelling and Simulation in Materials Science and Engineering, 2015, 23, 045001.	2.0	26
20	Size and shape of oxygen vacancies and protons in acceptor-doped barium zirconate. Solid State Ionics, 2015, 275, 2-8.	2.7	60
21	A computational study of special grain boundaries in WCâ€“Co cemented carbides. Computational Materials Science, 2015, 98, 345-353.	3.0	19
22	Oxygen vacancy segregation in grain boundaries of BaZrO3 using interatomic potentials. Solid State Ionics, 2013, 230, 27-31.	2.7	28
23	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
24	Oxygen vacancy segregation and space-charge effects in grain boundaries of dry and hydrated BaZrO3. Applied Physics Letters, 2012, 100, .	3.3	52
25	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
26	Transition Metal Solubilities in WC in Cemented Carbide Materials. Journal of the American Ceramic Society, 2011, 94, 605-610.	3.8	45
27	Theory of ultrathin films at metalâ€“ceramic interfaces. Philosophical Magazine Letters, 2010, 90, 599-609.	1.2	23
28	Using Neutron Spinâ^'Echo To Investigate Proton Dynamics in Proton-Conducting Perovskites. Chemistry of Materials, 2010, 22, 740-742.	6.7	43
29	Effective magnetic moment of magnetic multicore nanoparticles. Physical Review B, 2009, 80, .	3.2	50
30	Motion of nanometer sized magnetic particles in a magnetic field gradient. Journal of Applied Physics, 2008, 104, .	2.5	72
31	Path Integral Treatment of Proton Transport Processes inBaZrO3. Physical Review Letters, 2008, 101, 215902.	7.8	45
32	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
33	Structure and thermodynamic stability of hydrogen interstitials in BaZrO3perovskite oxide from density functional calculations. Faraday Discussions, 2007, 134, 247-265.	3.2	116
34	Early stages of phase separation using three-dimensional atom probe and atomistic modelling. Surface and Interface Analysis, 2007, 39, 178-183.	1.8	7
35	Thermodynamics of doping and vacancy formation inBaZrO3perovskite oxide from density functional calculations. Physical Review B, 2006, 73, .	3.2	139
36	Quantitative Analysis of WC Grain Shape in Sintered WC-Co Cemented Carbides. Physical Review Letters, 2005, 94, 066105.	7.8	48

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37	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
38	Motion of â€˜â€˜hotâ€™â€™ oxygen adatoms on corrugated metal surfaces. Journal of Chemical Physics, 1996, 105, 326-336.	3.0	85
39	H Motion in Pd and Nb: A Molecular-Dynamics Study. Materials Research Society Symposia Proceedings, 1992, 291, 537.	0.1	0