Daniel Scheiber

List of Publications by Year
in descending order

32	874	471371 17	477173 29
papers	citations	h-index	g-index

33	33	33	464
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Bond strength between TiN coating and microstructural constituents of a high speed steel determined by first principle calculations. Acta Materialia, 2022, 222, 117439.	3.8	17
2	Solute drag assessment of grain boundary migration in Au. Acta Materialia, 2022, 224, 117473.	3.8	16
3	Prediction of grain boundary chemistry in multicomponent Mo alloys with coupled precipitation and segregation kinetics simulations. Acta Materialia, 2022, 224, 117482.	3.8	4
4	Understanding and controlling inversion boundaries in ZnO. Acta Materialia, 2022, 229, 117804.	3.8	5
5	The segregation of transition metals to iron grain boundaries and their effects on cohesion. Acta Materialia, 2022, 231, 117902.	3.8	26
6	Selected Topics on Integrated Computational Material, Process, and Product Engineering. BHM-Zeitschrift Fuer Rohstoffe Geotechnik Metallurgie Werkstoffe Maschinen-Und Anlagentechnik, 2022, 167, 10-14.	0.4	1
7	Applications of Data Driven Methods in Computational Materials Design. BHM-Zeitschrift Fuer Rohstoffe Geotechnik Metallurgie Werkstoffe Maschinen-Und Anlagentechnik, 2022, 167, 29-35.	0.4	1
8	Solubility and segregation of B in paramagnetic fcc Fe. Physical Review Materials, 2022, 6, .	0.9	4
9	Hydrogen assisted intergranular cracking of alloy 725: The effect of boron and copper alloying. Corrosion Science, 2022, 203, 110331.	3.0	8
10	Analysis of shape, orientation and interface properties of Mo<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" altimg="si15.svg"><mml:msub><mml:mrow /><mml:mn>2</mml:mn></mml:msub></mml:math>C precipitates in Fe using ab-initio and finite element method calculations. Acta Materialia, 2021, 204, 116478.	3.8	8
11	Surface and segregation energies of Ag based alloys with Ni, Co and Fe: Direct experimental measurement and DFT study. Acta Materialia, 2021, 205, 116565.	3.8	17
12	Segregation and embrittlement of gold grain boundaries. Computational Materials Science, 2021, 187, 110110.	1.4	13
13	Grain boundary segregation in Ni-base alloys: A combined atom probe tomography and first principles study. Acta Materialia, 2021, 221, 117354.	3.8	37
14	Aluminum depletion induced by co-segregation of carbon and boron in a bcc-iron grain boundary. Nature Communications, 2021, 12, 6008.	5.8	24
15	Impact of the segregation energy spectrum on the enthalpy and entropy of segregation. Acta Materialia, 2021, 221, 117393.	3.8	23
16	Stainless steel reveals an anomaly in thermal expansion behavior of severely deformed materials. Physical Review Materials, 2021, 5, .	0.9	0
17	An understanding of hydrogen embrittlement in nickel grain boundaries from first principles. Materials and Design, 2021, 212, 110283.	3.3	20
18	On solute depletion zones along grain boundaries during segregation. Acta Materialia, 2020, 182, 100-107.	3.8	14

#	Article	IF	Citations
19	Hydrogen-enhanced intergranular failure of sulfur-doped nickel grain boundary: In situ electrochemical micro-cantilever bending vs.ÂDFT. Materials Science & Engineering A: Structural Materials: Properties, Microstructure and Processing, 2020, 794, 139967.	2.6	27
20	Temperature dependence of surface and grain boundary energies from first principles. Physical Review B, 2020, 101, .	1.1	26
21	Hydrogen Trapping in bcc Iron. Materials, 2020, 13, 2288.	1.3	42
22	The influence of alloying on Zn liquid metal embrittlement in steels. Acta Materialia, 2020, 195, 750-760.	3.8	45
23	Morphology of Fe2Al5 particles and the interface to WC coating in the context of hot-dip galvanizing: An ab initio study. Journal of Alloys and Compounds, 2020, 824, 153854.	2.8	16
24	How grain boundary chemistry controls the fracture mode of molybdenum. Materials and Design, 2018, 142, 36-43.	3.3	52
25	Kinetics of grain boundary segregation in multicomponent systems â€“ The example of a Mo-C-B-O system. Scripta Materialia, 2018, 150, 110-114.	2.6	22
26	New Cr-Ni-Base Alloy for High-Temperature Applications Designed on the Basis of First Principles Calculations. Advances in Condensed Matter Physics, 2018, 2018, 1-8.	0.4	13
27	Impact of solute-solute interactions on grain boundary segregation and cohesion in molybdenum. Physical Review Materials, 2018, 2, .	0.9	19
28	Ab-initio search for cohesion-enhancing solute elements at grain boundaries in molybdenum and tungsten. International Journal of Refractory Metals and Hard Materials, 2016, 60, 75-81.	1.7	82
29	Ab initiosearch for cohesion-enhancing impurity elements at grain boundaries in molybdenum and tungsten. Modelling and Simulation in Materials Science and Engineering, 2016, 24, 085009.	0.8	57
30	Ab initiocalculations of grain boundaries in bcc metals. Modelling and Simulation in Materials Science and Engineering, 2016, 24, 035013.	0.8	113
31	The roles of Eu during the growth of eutectic Si in Al-Si alloys. Scientific Reports, 2015, 5, 13802.	1.6	35
32	Ab initio description of segregation and cohesion of grain boundaries in Wâ€“25 at.% Re alloys. Acta Materialia, 2015, 88, 180-189.	3.8	87