

Lorenz Romaner

List of Publications by Citations

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The third column is the impact factor (IF) of the journal, and the fourth column is the number of citations of the article.

74
papers

4,187
citations

30
h-index

64
g-index

81
ext. papers

4,616
ext. citations

6.2
avg, IF

5.23
L-index

#	Paper	IF	Citations
74	Recent progress in research on tungsten materials for nuclear fusion applications in Europe. <i>Journal of Nuclear Materials</i> , 2013 , 432, 482-500	3.3	494
73	The interface energetics of self-assembled monolayers on metals. <i>Accounts of Chemical Research</i> , 2008 , 41, 721-9	24.3	340
72	Van der Waals Interactions Between Organic Adsorbates and at Organic/Inorganic Interfaces. <i>MRS Bulletin</i> , 2010 , 35, 435-442	3.2	244
71	Toward control of the metal-organic interfacial electronic structure in molecular electronics: a first-principles study on self-assembled monolayers of pi-conjugated molecules on noble metals. <i>Nano Letters</i> , 2007 , 7, 932-40	11.5	244
70	Interface energetics and level alignment at covalent metal-molecule junctions: pi-conjugated thiols on gold. <i>Physical Review Letters</i> , 2006 , 96, 196806	7.4	243
69	The Origin of Green Emission in Polyfluorene-Based Conjugated Polymers: On-Chain Defect Fluorescence. <i>Advanced Functional Materials</i> , 2003 , 13, 597-601	15.6	243
68	Effect of rhenium on the dislocation core structure in tungsten. <i>Physical Review Letters</i> , 2010 , 104, 195503	7.4	192
67	Impact of bidirectional charge transfer and molecular distortions on the electronic structure of a metal-organic interface. <i>Physical Review Letters</i> , 2007 , 99, 256801	7.4	186
66	Theoretical study of PTCDA adsorbed on the coinage metal surfaces, Ag(111), Au(111) and Cu(111). <i>New Journal of Physics</i> , 2009 , 11, 053010	2.9	175
65	Review on the EFDA programme on tungsten materials technology and science. <i>Journal of Nuclear Materials</i> , 2011 , 417, 463-467	3.3	139
64	Organic/metal interfaces in self-assembled monolayers of conjugated thiols: A first-principles benchmark study. <i>Surface Science</i> , 2006 , 600, 4548-4562	1.8	122
63	F4TCNQ on Cu, Ag, and Au as prototypical example for a strong organic acceptor on coinage metals. <i>Physical Review B</i> , 2009 , 79,	3.3	108
62	The Dielectric Constant of Self-Assembled Monolayers. <i>Advanced Functional Materials</i> , 2008 , 18, 3999-4006	10.66	95
61	Dislocation-core symmetry and slip planes in tungsten alloys: Ab initio calculations and microcantilever bending experiments. <i>Acta Materialia</i> , 2012 , 60, 748-758	8.4	91
60	Orbital tomography: Deconvoluting photoemission spectra of organic molecules. <i>Physical Review B</i> , 2011 , 84,	3.3	86
59	Ab initio calculations of grain boundaries in bcc metals. <i>Modelling and Simulation in Materials Science and Engineering</i> , 2016 , 24, 035013	2	77
58	Electronic structure of thiol-bonded self-assembled monolayers: Impact of coverage. <i>Physical Review B</i> , 2008 , 77,	3.3	71

57	Odd-even effects in self-assembled monolayers of omega-(biphenyl-4-yl)alkanethiols: a first-principles study. <i>Langmuir</i> , 2008 , 24, 474-82	4	69
56	Ab initio description of segregation and cohesion of grain boundaries in W ₅ at.% Re alloys. <i>Acta Materialia</i> , 2015 , 88, 180-189	8.4	67
55	A brief summary of the progress on the EFDA tungsten materials program. <i>Journal of Nuclear Materials</i> , 2013 , 442, S173-S180	3.3	63
54	Epitaxy of rodlike organic molecules on sheet silicates--a growth model based on experiments and simulations. <i>Journal of the American Chemical Society</i> , 2011 , 133, 3056-62	16.4	59
53	Ketonic Defects in Ladder-type Poly(p-phenylene)s. <i>Chemistry of Materials</i> , 2004 , 16, 4667-4674	9.6	47
52	Ab-initio search for cohesion-enhancing solute elements at grain boundaries in molybdenum and tungsten. <i>International Journal of Refractory Metals and Hard Materials</i> , 2016 , 60, 75-81	4.1	46
51	Stretching and breaking of a molecular junction. <i>Small</i> , 2006 , 2, 1468-75	11	40
50	Understanding the properties of interfaces between organic self-assembled monolayers and noble metals— theoretical perspective. <i>Surface and Interface Analysis</i> , 2008 , 40, 371-378	1.5	39
49	Ab initio search for cohesion-enhancing impurity elements at grain boundaries in molybdenum and tungsten. <i>Modelling and Simulation in Materials Science and Engineering</i> , 2016 , 24, 085009	2	38
48	First-principles study of the geometric and electronic structure of Au ₁₃ clusters: Importance of the prism motif. <i>Physical Review B</i> , 2008 , 77,	3.3	38
47	Electronic Structure of Self-Assembled Monolayers on Au(111) Surfaces: The Impact of Backbone Polarizability. <i>Advanced Functional Materials</i> , 2009 , 19, 3766-3775	15.6	36
46	The electronic structure of mixed self-assembled monolayers. <i>ACS Nano</i> , 2010 , 4, 6735-46	16.7	34
45	Simultaneously Understanding the Geometric and Electronic Structure of Anthraceneselenolate on Au(111): A Combined Theoretical and Experimental Study. <i>Journal of Physical Chemistry C</i> , 2010 , 114, 2677-2684	3.8	32
44	Doping molecular wires. <i>Nano Letters</i> , 2009 , 9, 2559-64	11.5	29
43	How grain boundary chemistry controls the fracture mode of molybdenum. <i>Materials and Design</i> , 2018 , 142, 36-43	8.1	28
42	A momentum space view of the surface chemical bond. <i>Physical Chemistry Chemical Physics</i> , 2011 , 13, 3604-11	3.6	26
41	The roles of Eu during the growth of eutectic Si in Al-Si alloys. <i>Scientific Reports</i> , 2015 , 5, 13802	4.9	25
40	Comparison of thermal and electrical degradation effects in polyfluorenes. <i>Synthetic Metals</i> , 2003 , 139, 855-858	3.6	25

39	Solute segregation in Cu: DFT vs. Experiment. <i>Acta Materialia</i> , 2018 , 147, 122-132	8.4	24
38	Comprehensive photophysical studies of polyfluorenes containing on-chain emissive defects. <i>Physical Review B</i> , 2005 , 72,	3.3	22
37	Hydrogen Trapping in bcc Iron. <i>Materials</i> , 2020 , 13,	3.5	20
36	Improving the Stability of Polymer FETs by Introducing Fixed Acceptor Units into the Main Chain: Application to Poly(alkylthiophenes). <i>Chemistry of Materials</i> , 2007 , 19, 1472-1481	9.6	20
35	The Effect of Protonation on the Optical Properties of Conjugated FluorenePyridine Copolymers. <i>Macromolecular Chemistry and Physics</i> , 2008 , 209, 2122-2134	2.6	18
34	The influence of keto defects on photoexcitation dynamics in polyfluorene. <i>Synthetic Metals</i> , 2003 , 139, 851-854	3.6	18
33	Response modeling of single SnO ₂ nanowire gas sensors. <i>Sensors and Actuators B: Chemical</i> , 2019 , 295, 22-29	8.5	16
32	Impact of d-band filling on the dislocation properties of bcc transition metals: The case of tantalum-tungsten alloys investigated by density-functional theory. <i>Physical Review B</i> , 2017 , 95,	3.3	15
31	Temperature dependence of surface and grain boundary energies from first principles. <i>Physical Review B</i> , 2020 , 101,	3.3	14
30	Kinetics of grain boundary segregation in multicomponent systems – The example of a Mo-C-B-O system. <i>Scripta Materialia</i> , 2018 , 150, 110-114	5.6	14
29	Core polarity of screw dislocations in FeTi alloys. <i>Philosophical Magazine Letters</i> , 2014 , 94, 334-341	1	14
28	The influence of alloying on Zn liquid metal embrittlement in steels. <i>Acta Materialia</i> , 2020 , 195, 750-760	8.4	12
27	Impact of solute-solute interactions on grain boundary segregation and cohesion in molybdenum. <i>Physical Review Materials</i> , 2018 , 2,	3.2	11
26	Thermal expansion coefficient of WRe alloys from first principles. <i>Physical Review B</i> , 2017 , 96,	3.3	10
25	Analysis of Bonding between Conjugated Organic Molecules and Noble Metal Surfaces Using Orbital Overlap Populations. <i>Journal of Chemical Theory and Computation</i> , 2010 , 6, 3481-3489	6.4	9
24	Verification of the generalised chemical potential for stress-driven hydrogen diffusion in nickel. <i>Philosophical Magazine Letters</i> , 2020 , 100, 513-523	1	7
23	On solute depletion zones along grain boundaries during segregation. <i>Acta Materialia</i> , 2020 , 182, 100-107	8.4	7
22	A theoretical view on self-assembled monolayers in organic electronic devices 2008 ,		6

21	Hydrogen segregation near a crack tip in nickel. <i>Scripta Materialia</i> , 2021 , 194, 113697	5.6	6
20	Ab Initio Study of Elastic and Mechanical Properties in FeCrMn Alloys. <i>Materials</i> , 2019 , 12,	3.5	5
19	Aluminum depletion induced by co-segregation of carbon and boron in a bcc-iron grain boundary. <i>Nature Communications</i> , 2021 , 12, 6008	17.4	4
18	Study on Ca Segregation toward an Epitaxial Interface between Bismuth Ferrite and Strontium Titanate. <i>ACS Applied Materials & Interfaces</i> , 2020 , 12, 12264-12274	9.5	3
17	A detailed study of the photophysics of organic semiconducting nanospheres. <i>Synthetic Metals</i> , 2003 , 139, 609-612	3.6	3
16	Ab initio Calculations as a Tool for Predicting Materials Properties. <i>BHM-Zeitschrift Fuer Rohstoffe Geotechnik Metallurgie Werkstoffe Maschinen-Und Anlagentechnik</i> , 2014 , 159, 367-370	0.6	2
15	Deviations and polarity of [100] dislocations in bcc metals. <i>Philosophical Magazine Letters</i> , 2010 , 90, 385-391	2	2
14	Impact of the segregation energy spectrum on the enthalpy and entropy of segregation. <i>Acta Materialia</i> , 2021 , 221, 117393	8.4	2
13	The influence of chemistry on the interface toughness in a WTi-Cu system. <i>Acta Materialia</i> , 2022 , 230, 117813	8.4	2
12	Energies and structures of Cu/Nb and Cu/W interfaces from density functional theory and semi-empirical calculations. <i>Materialia</i> , 2022 , 101362	3.2	1
11	Solute drag assessment of grain boundary migration in Au. <i>Acta Materialia</i> , 2021 , 117473	8.4	1
10	An understanding of hydrogen embrittlement in nickel grain boundaries from first principles. <i>Materials and Design</i> , 2021 , 212, 110283	8.1	1
9	Solubility and segregation of B in paramagnetic fcc Fe. <i>Physical Review Materials</i> , 2022 , 6,	3.2	1
8	Prediction of grain boundary chemistry in multicomponent Mo alloys with coupled precipitation and segregation kinetics simulations. <i>Acta Materialia</i> , 2021 , 224, 117482	8.4	0
7	Bond strength between TiN coating and microstructural constituents of a high speed steel determined by first principle calculations. <i>Acta Materialia</i> , 2021 , 117439	8.4	0
6	Theoretical investigation of the 70.5° mixed dislocations in body-centered cubic transition metals. <i>Acta Materialia</i> , 2021 , 217, 117154	8.4	0
5	The segregation of transition metals to iron grain boundaries and their effects on cohesion. <i>Acta Materialia</i> , 2022 , 231, 117902	8.4	0
4	Applications of Data Driven Methods in Computational Materials Design. <i>BHM-Zeitschrift Fuer Rohstoffe Geotechnik Metallurgie Werkstoffe Maschinen-Und Anlagentechnik</i> , 2022 , 167, 29-35	0.6	0

3	Tuning mechanical properties of ultrafine-grained tungsten by manipulating grain boundary chemistry. <i>Acta Materialia</i> , 2022 , 117939	8.4	o
2	Ca Solubility in a BiFeO-Based System with a Secondary BiO Phase on a Nanoscale.. <i>Journal of Physical Chemistry C</i> , 2022 , 126, 7696-7703	3.8	o
1	Organic/Organic Heteroepitaxy: The Method of Choice to Tune Optical Emission of Organic Nano-fibers?. <i>Springer Series in Materials Science</i> , 2013 , 49-78	0.9	