Lorenz Romaner

List of Publications by Year in Descending Order

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	Energies and structures of Cu/Nb and Cu/W interfaces from density functional theory and semi-empirical calculations. *Materialia*, **2022**, 101362	3.2	1
73	The influence of chemistry on the interface toughness in a WTi-Cu system. *Acta Materialia*, **2022**, 230, 117813	8.4	2
72	The segregation of transition metals to iron grain boundaries and their effects on cohesion. *Acta Materialia*, **2022**, 231, 117902	8.4	0
71	Applications of Data Driven Methods in Computational Materials Design. *BHM-Zeitschrift Fuer Rohstoffe Geotechnik Metallurgie Werkstoffe Maschinen-Und Anlagentechnik*, **2022**, 167, 29-35	0.6	0
70	Tuning mechanical properties of ultrafine-grained tungsten by manipulating grain boundary chemistry. *Acta Materialia*, **2022**, 117939	8.4	0
69	Solubility and segregation of B in paramagnetic fcc Fe. *Physical Review Materials*, **2022**, 6,	3.2	1
68	Ca Solubility in a BiFeO-Based System with a Secondary BiO Phase on a Nanoscale.. *Journal of Physical Chemistry C*, **2022**, 126, 7696-7703	3.8	0
67	Solute drag assessment of grain boundary migration in Au. *Acta Materialia*, **2021**, 117473	8.4	1
66	Prediction of grain boundary chemistry in multicomponent Mo alloys with coupled precipitation and segregation kinetics simulations. *Acta Materialia*, **2021**, 224, 117482	8.4	0
65	An understanding of hydrogen embrittlement in nickel grain boundaries from first principles. *Materials and Design*, **2021**, 212, 110283	8.1	1
64	Bond strength between TiN coating and microstructural constituents of a high speed steel determined by first principle calculations. *Acta Materialia*, **2021**, 117439	8.4	0
63	Aluminum depletion induced by co-segregation of carbon and boron in a bcc-iron grain boundary. *Nature Communications*, **2021**, 12, 6008	17.4	4
62	Impact of the segregation energy spectrum on the enthalpy and entropy of segregation. *Acta Materialia*, **2021**, 221, 117393	8.4	2
61	Hydrogen segregation near a crack tip in nickel. *Scripta Materialia*, **2021**, 194, 113697	5.6	6
60	Theoretical investigation of the 70.5°mixed dislocations in body-centered cubic transition metals. *Acta Materialia*, **2021**, 217, 117154	8.4	0
59	Temperature dependence of surface and grain boundary energies from first principles. *Physical Review B*, **2020**, 101,	3.3	14
58	Hydrogen Trapping in bcc Iron. *Materials*, **2020**, 13,	3.5	20

57	The influence of alloying on Zn liquid metal embrittlement in steels. *Acta Materialia*, **2020**, 195, 750-760	8.4	12
56	Study on Ca Segregation toward an Epitaxial Interface between Bismuth Ferrite and Strontium Titanate. *ACS Applied Materials & Interfaces*, **2020**, 12, 12264-12274	9.5	3
55	Verification of the generalised chemical potential for stress-driven hydrogen diffusion in nickel. *Philosophical Magazine Letters*, **2020**, 100, 513-523	1	7
54	On solute depletion zones along grain boundaries during segregation. *Acta Materialia*, **2020**, 182, 100-107	8.4	7
53	Response modeling of single SnO2 nanowire gas sensors. *Sensors and Actuators B: Chemical*, **2019**, 295, 22-29	8.5	16
52	Ab Initio Study of Elastic and Mechanical Properties in FeCrMn Alloys. *Materials*, **2019**, 12,	3.5	5
51	Solute segregation in Cu: DFT vs. Experiment. *Acta Materialia*, **2018**, 147, 122-132	8.4	24
50	How grain boundary chemistry controls the fracture mode of molybdenum. *Materials and Design*, **2018**, 142, 36-43	8.1	28
49	Kinetics of grain boundary segregation in multicomponent systems The example of a Mo-C-B-O system. *Scripta Materialia*, **2018**, 150, 110-114	5.6	14
48	Impact of solute-solute interactions on grain boundary segregation and cohesion in molybdenum. *Physical Review Materials*, **2018**, 2,	3.2	11
47	Impact of d-band filling on the dislocation properties of bcc transition metals: The case of tantalum-tungsten alloys investigated by density-functional theory. *Physical Review B*, **2017**, 95,	3.3	15
46	Thermal expansion coefficient of WRe alloys from first principles. *Physical Review B*, **2017**, 96,	3.3	10
45	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	2	38
44	Ab initiocalculations of grain boundaries in bcc metals. *Modelling and Simulation in Materials Science and Engineering*, **2016**, 24, 035013	2	77
43	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	4.1	46
42	The roles of Eu during the growth of eutectic Si in Al-Si alloys. *Scientific Reports*, **2015**, 5, 13802	4.9	25
41	Ab initio description of segregation and cohesion of grain boundaries in W25 at.% Re alloys. *Acta Materialia*, **2015**, 88, 180-189	8.4	67
40	Core polarity of screw dislocations in FeCo alloys. *Philosophical Magazine Letters*, **2014**, 94, 334-341	1	14

39	Ab initio Calculations as a Tool for Predicting Materials Properties. *BHM-Zeitschrift Fuer Rohstoffe Geotechnik Metallurgie Werkstoffe Maschinen-Und Anlagentechnik*, **2014**, 159, 367-370	0.6	2
38	A brief summary of the progress on the EFDA tungsten materials program. *Journal of Nuclear Materials*, **2013**, 442, S173-S180	3.3	63
37	Organic□Organic Heteroepitaxy□The Method of Choice to Tune Optical Emission of Organic Nano-fibers?. *Springer Series in Materials Science*, **2013**, 49-78	0.9	
36	Recent progress in research on tungsten materials for nuclear fusion applications in Europe. *Journal of Nuclear Materials*, **2013**, 432, 482-500	3.3	494
35	Dislocation-core symmetry and slip planes in tungsten alloys: Ab initio calculations and microcantilever bending experiments. *Acta Materialia*, **2012**, 60, 748-758	8.4	91
34	Review on the EFDA programme on tungsten materials technology and science. *Journal of Nuclear Materials*, **2011**, 417, 463-467	3.3	139
33	A momentum space view of the surface chemical bond. *Physical Chemistry Chemical Physics*, **2011**, 13, 3604-11	3.6	26
32	Epitaxy of rodlike organic molecules on sheet silicates--a growth model based on experiments and simulations. *Journal of the American Chemical Society*, **2011**, 133, 3056-62	16.4	59
31	Orbital tomography: Deconvoluting photoemission spectra of organic molecules. *Physical Review B*, **2011**, 84,	3.3	86
30	The electronic structure of mixed self-assembled monolayers. *ACS Nano*, **2010**, 4, 6735-46	16.7	34
29	Simultaneously Understanding the Geometric and Electronic Structure of Anthraceneselenolate on Au(111): A Combined Theoretical and Experimental Study. *Journal of Physical Chemistry C*, **2010**, 114, 2677-2684	3.8	32
28	Analysis of Bonding between Conjugated Organic Molecules and Noble Metal Surfaces Using Orbital Overlap Populations. *Journal of Chemical Theory and Computation*, **2010**, 6, 3481-3489	6.4	9
27	Deviations and polarity of [100] dislocations in bcc metals. *Philosophical Magazine Letters*, **2010**, 90, 385-391	1	2
26	Van der Waals Interactions Between Organic Adsorbates and at Organic/Inorganic Interfaces. *MRS Bulletin*, **2010**, 35, 435-442	3.2	244
25	Effect of rhenium on the dislocation core structure in tungsten. *Physical Review Letters*, **2010**, 104, 195503	7.4	192
24	F4TCNQ on Cu, Ag, and Au as prototypical example for a strong organic acceptor on coinage metals. *Physical Review B*, **2009**, 79,	3.3	108
23	Electronic Structure of Self-Assembled Monolayers on Au(111) Surfaces: The Impact of Backbone Polarizability. *Advanced Functional Materials*, **2009**, 19, 3766-3775	15.6	36
22	Theoretical study of PTCDA adsorbed on the coinage metal surfaces, Ag(111), Au(111) and Cu(111). *New Journal of Physics*, **2009**, 11, 053010	2.9	175

21	Doping molecular wires. *Nano Letters*, **2009**, 9, 2559-64	11.5	29
20	The interface energetics of self-assembled monolayers on metals. *Accounts of Chemical Research*, **2008**, 41, 721-9	24.3	340
19	First-principles study of the geometric and electronic structure of Au13 clusters: Importance of the prism motif. *Physical Review B*, **2008**, 77,	3.3	38
18	Odd-even effects in self-assembled monolayers of omega-(biphenyl-4-yl)alkanethiols: a first-principles study. *Langmuir*, **2008**, 24, 474-82	4	69
17	A theoretical view on self-assembled monolayers in organic electronic devices **2008**,		6
16	Electronic structure of thiol-bonded self-assembled monolayers: Impact of coverage. *Physical Review B*, **2008**, 77,	3.3	71
15	Understanding the properties of interfaces between organic self-assembled monolayers and noble metals□ theoretical perspective. *Surface and Interface Analysis*, **2008**, 40, 371-378	1.5	39
14	The Effect of Protonation on the Optical Properties of Conjugated Fluorene□Pyridine Copolymers. *Macromolecular Chemistry and Physics*, **2008**, 209, 2122-2134	2.6	18
13	The Dielectric Constant of Self-Assembled Monolayers. *Advanced Functional Materials*, **2008**, 18, 3999-4006	15.6	95
12	Improving the Stability of Polymer FETs by Introducing Fixed Acceptor Units into the Main Chain: Application to Poly(alkylthiophenes). *Chemistry of Materials*, **2007**, 19, 1472-1481	9.6	20
11	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. *Nano Letters*, **2007**, 7, 932-40	11.5	244
10	Impact of bidirectional charge transfer and molecular distortions on the electronic structure of a metal-organic interface. *Physical Review Letters*, **2007**, 99, 256801	7.4	186
9	Organic/metal interfaces in self-assembled monolayers of conjugated thiols: A first-principles benchmark study. *Surface Science*, **2006**, 600, 4548-4562	1.8	122
8	Interface energetics and level alignment at covalent metal-molecule junctions: pi-conjugated thiols on gold. *Physical Review Letters*, **2006**, 96, 196806	7.4	243
7	Stretching and breaking of a molecular junction. *Small*, **2006**, 2, 1468-75	11	40
6	Comprehensive photophysical studies of polyfluorenes containing on-chain emissive defects. *Physical Review B*, **2005**, 72,	3.3	22
5	Ketonic Defects in Ladder-type Poly(p-phenylene)s. *Chemistry of Materials*, **2004**, 16, 4667-4674	9.6	47
4	The Origin of Green Emission in Polyfluorene-Based Conjugated Polymers: On-Chain Defect Fluorescence. *Advanced Functional Materials*, **2003**, 13, 597-601	15.6	243

3	A detailed study of the photophysics of organic semiconducting nanospheres. *Synthetic Metals*, **2003**, 139, 609-612	3.6	3
2	The influence of keto defects on photoexcitation dynamics in polyfluorene. *Synthetic Metals*, **2003**, 139, 851-854	3.6	18
1	Comparison of thermal and electrical degradation effects in polyfluorenes. *Synthetic Metals*, **2003**, 139, 855-858	3.6	25