Marian Krajci

List of Publications by Citations

116 papers	2,424 citations	31 h-index	44 g-index
120 ext. papers	2,544 ext. citations	3.5 avg, IF	5.09 L-index

#	Paper	IF	Citations
116	Electronic structure and stability of quasicrystals: Quasiperiodic dispersion relations and pseudogaps. *Physical Review Letters*, **1992**, 68, 2321-2324	7.4	124
115	Shear deformation, ideal strength, and stacking fault formation of fcc metals: A density-functional study of Al and Cu. *Physical Review B*, **2009**, 79,	3.3	120
114	Atomic and electronic structure of icosahedral Al-Pd-Mn alloys and approximant phases. *Physical Review B*, **1995**, 51, 17355-17378	3.3	118
113	Electronic structure of quasicrystalline Al-Zn-Mg alloys and related crystalline, amorphous, and liquid phases. *Physical Review B*, **1993**, 47, 11795-11809	3.3	70
112	Interatomic bonding, elastic properties, and ideal strength of transition metal aluminides: A case study for Al3(V,Ti). *Physical Review B*, **2005**, 71,	3.3	61
111	Formation of magnetic moments in crystalline, quasicrystalline, and liquid Al-Mn alloys. *Physical Review B*, **1998**, 57, 2849-2860	3.3	59
110	Structure, stability, and electronic properties of the i-AlPdMn quasicrystalline surface. *Physical Review B*, **2005**, 71,	3.3	57
109	Ordered structures in rhenium binary alloys from first-principles calculations. *Journal of the American Chemical Society*, **2011**, 133, 158-63	16.4	53
108	Complex intermetallic compounds as selective hydrogenation catalysts A case study for the (100) surface of Al13Co4. *Journal of Catalysis*, **2011**, 278, 200-207	7.3	52
107	Anomalies in the response of V, Nb, and Ta to tensile and shear loading: Ab initio density functional theory calculations. *Physical Review B*, **2010**, 81,	3.3	50
106	Propagating and confined vibrational excitations in quasicrystals. *Journal of Physics Condensed Matter*, **1993**, 5, 2489-2510	1.8	48
105	Surface vacancies at the fivefold icosahedral Al-Pd-Mn quasicrystal surface: A comparison of ab initio calculated and experimental STM images. *Physical Review B*, **2006**, 73,	3.3	47
104	Ordered phases in ruthenium binary alloys from high-throughput first-principles calculations. *Physical Review B*, **2011**, 84,	3.3	43
103	Covalent bonding and bandgap formation in transition-metal aluminides: di-aluminides of group VIII transition metals. *Journal of Physics Condensed Matter*, **2002**, 14, 5755-5783	1.8	41
102	The (2 1 0) surface of intermetallic B20 compound GaPd as a selective hydrogenation catalyst: A DFT study. *Journal of Catalysis*, **2012**, 295, 70-80	7.3	40
101	Intermetallic Compound AlPd As a Selective Hydrogenation Catalyst: A DFT Study. *Journal of Physical Chemistry C*, **2012**, 116, 6307-6319	3.8	40
100	Electronic structure and transport properties of decagonal Al-Cu-Co alloys. *Physical Review B*, **1997**, 56, 3072-3085	3.3	40

99	Structure and lattice dynamics of rational approximants to icosahedral Al-Cu-Li. *Physical Review B*, **1994**, 49, 8701-8717	3.3	40
98	Selective semi-hydrogenation of acetylene: Atomistic scenario for reactions on the polar threefold surfaces of GaPd. *Journal of Catalysis*, **2014**, 312, 232-248	7.3	39
97	Atomic and electronic structure of decagonal Al-Pd-Mn alloys and approximant phases. *Physical Review B*, **1997**, 55, 843-855	3.3	39
96	Ab initio study of quasiperiodic monolayers on a fivefold i-AlPdMn surface. *Physical Review B*, **2005**, 71,	3.3	39
95	Intermetallic Compounds as Selective Heterogeneous Catalysts: Insights from DFT. *ChemCatChem*, **2016**, 8, 34-48	5.2	38
94	Nucleation of Pb starfish clusters on the five-fold Al-Pd-Mn quasicrystal surface. *Physical Review B*, **2009**, 79,	3.3	37
93	Covalent bonding and bandgap formation in intermetallic compounds: a case study for Al3V. *Journal of Physics Condensed Matter*, **2002**, 14, 1865-1879	1.8	37
92	Strictly localized eigenstates on a three-dimensional Penrose lattice. *Physical Review B*, **1988**, 38, 12903-12907	3.3	37
91	Temperature-induced martensitic phase transitions in gum-metal approximants: First-principles investigations for Ti3Nb. *Physical Review B*, **2011**, 84,	3.3	36
90	Ab initio study of the surface of a decagonal Al-Co-Ni quasicrystal. *Physical Review B*, **2006**, 73,	3.3	36
89	Structure and stability of quasicrystals: Modulated tiling models. *Physical Review B*, **1992**, 46, 10669-10685	3.3	35
88	Propagating and localized vibrational modes in Ni-Zr glasses. *Journal of Physics Condensed Matter*, **1994**, 6, 4631-4654	1.8	34
87	Atomic and electronic structure of decagonal Al-Ni-Co alloys and approximant phases. *Physical Review B*, **2000**, 62, 243-255	3.3	33
86	Propagating and localized elementary excitations in decagonal quasicrystals. *Physical Review Letters*, **1996**, 76, 2738-2741	7.4	32
85	Electronic Structure of Rational Approximants to Icosahedral Quasi-Crystals. *Europhysics Letters*, **1992**, 17, 145-150	1.6	30
84	Electronic structure in icosahedral AlCuLi quasicrystals and approximant crystals. *Journal of Physics Condensed Matter*, **1994**, 6, 6977-6995	1.8	29
83	Computer Simulation of Frank-Kasper-Type Icosahedral Quasi-Crystals. *Europhysics Letters*, **1990**, 13, 335-340	1.6	27
82	Understanding the selectivity of methanol steam reforming on the (1 1 1) surfaces of NiZn, PdZn and PtZn: Insights from DFT. *Journal of Catalysis*, **2015**, 330, 6-18	7.3	26

81	Semihydrogenation of Acetylene on the (010) Surface of GaPd2: Ga Enrichment Improves Selectivity. *Journal of Physical Chemistry C*, **2014**, 118, 12285-12301	3.8	26
80	Isolated magnetic moments in icosahedral Al-Pd-Mn alloys. *Physical Review B*, **1998**, 58, 14110-14112	3.3	26
79	Semiconducting Al□ransition-metal quasicrystals. *Physical Review B*, **2003**, 68,	3.3	23
78	Structure of the (010) surface of the orthorhombic complex metallic alloy T-Al3(Mn,Pd). *Physical Review B*, **2010**, 81,	3.3	22
77	Metal-insulator transition in approximants to icosahedral Al-Pd-Re. *Physical Review B*, **1999**, 59, 8347-8350	3.3	22
76	Interatomic bonds and the tensile anisotropy of trialuminides in the elastic limit: a density functional study for Al3(Sc, Ti, V, Cr). *Philosophical Magazine*, **2007**, 87, 1769-1794	1.6	21
75	Response of trialuminides to [110] uniaxial loading: An ab initio study for Al3(Sc,Ti,V). *Physical Review B*, **2007**, 76,	3.3	21
74	Topologically induced semiconductivity in icosahedral Al-Pd-Re and its approximants. *Physical Review B*, **2007**, 75,	3.3	20
73	Structure and chemical reactivity of the polar three-fold surfaces of GaPd: a density-functional study. *Journal of Chemical Physics*, **2013**, 138, 124703	3.9	19
72	Surface structures of complex intermetallic compounds: An abinitio DFT study for the (100) surface of o-Al13Co4. *Physical Review B*, **2011**, 84,	3.3	19
71	Pseudomorphic quasiperiodic alkali metal monolayers on an iAlPdMn surface. *Physical Review B*, **2007**, 75,	3.3	19
70	Are decagonal quasicrystals stabilized by a Hume-Rothery mechanism?. *Europhysics Letters*, **1996**, 34, 207-212	1.6	19
69	Covalent bonding and band-gap formation in ternary transition-metal di-aluminides: Al4MnCo and related compounds. *Journal of Physics Condensed Matter*, **2002**, 14, 7201-7219	1.8	17
68	Propagating Collective Excitations in Quasi-Crystals. *Europhysics Letters*, **1993**, 21, 31-36	1.6	16
67	Surfaces of intermetallic compounds: An ab initio DFT study for B20-type AlPd. *Physical Review B*, **2013**, 87,	3.3	15
66	Quasiperiodic Pb monolayer on the fivefold i-Al-Pd-Mn surface: Structure and electronic properties. *Physical Review B*, **2010**, 82,	3.3	15
65	Structure, electronic density of states and electric field gradients of icosahedral AlCuFe: An ab initio study of the original and a modified Cockayne model. *Physical Review B*, **2004**, 69,	3.3	15
64	Twinning in fcc lattice creates low-coordinated catalytically active sites in porous gold. *Journal of Chemical Physics*, **2016**, 145, 084703	3.9	15

63	Surfaces of complex intermetallic compounds: insights from density functional calculations. *Accounts of Chemical Research*, **2014**, 47, 3378-84	24.3	14
62	Ab initio study of quasiperiodic Bi monolayers on a tenfold dAlCoNi surface. *Physical Review B*, **2006**, 73,	3.3	14
61	Highly anisotropic electronic structure in decagonal quasicrystals and approximants. *Physical Review B*, **1998**, 58, 5378-5383	3.3	14
60	Localized modes and topological frustration in rational approximants to quasicrystals. *Physical Review B*, **1993**, 47, 1084-1087	3.3	14
59	Understanding the catalytic activity of nanoporous gold: Role of twinning in fcc lattice. *Journal of Chemical Physics*, **2017**, 147, 044713	3.9	13
58	Thin Film Growth on Quasicrystalline Surfaces. *Israel Journal of Chemistry*, **2011**, 51, 1314-1325	3.4	13
57	Quasiperiodic layers of free-electron metals studied using electron diffraction. *Physical Review B*, **2009**, 79,	3.3	13
56	Fivefold iAlPdMn surface as template for growing monatomic quasiperiodic layers: First-principles simulations for adatoms from groups one to three. *Physical Review B*, **2008**, 77,	3.3	13
55	Electronic and magnetic properties of hexagonal rare-earth-Zn-Mg compounds and their relation to the properties of icosahedral alloys. *Journal of Physics Condensed Matter*, **2000**, 12, 5831-5842	1.8	13
54	"Fuzzy" tight-binding Monte Carlo method: A O(N) technique for calculating structural and electronic properties of materials. *Physical Review Letters*, **1995**, 74, 5100-5103	7.4	13
53	Fermi surfaces and electronic transport properties of quasicrystalline approximants. *Journal of Physics Condensed Matter*, **2001**, 13, 3817-3830	1.8	12
52	Electronic Structure of Approximant Phase to Icosahedral Ti-Transition-Metal Quasi-Crystals. *Europhysics Letters*, **1994**, 27, 147-152	1.6	12
51	Computer study of the dependence of the d-electronic structure of amorphous systems on their atomic structure. *Journal of Physics F: Metal Physics*, **1987**, 17, 2217-2234		11
50	Computer simulation of amorphous alloy Fe100-xBx, x=14-25. *Journal of Physics F: Metal Physics*, **1988**, 18, 2137-2147		11
49	Computer simulations of the structure of amorphous systems by the Markov chain method. *Journal of Physics F: Metal Physics*, **1984**, 14, 1325-1332		11
48	Highly selective semi-hydrogenation of acetylene over porous gold with twin boundary defects. *Applied Catalysis A: General*, **2019**, 569, 101-109	5.1	11
47	Synthetically Tuned Pd-Based Intermetallic Compounds and their Structural Influence on the O Dissociation in Benzylamine Oxidation. *ACS Applied Materials & Interfaces*, **2019**, 11, 37602-37616	9.5	10
46	Electronic and structural properties of Laves-phase MgZn2 of varying chemical disorder. *Physical Review B*, **2010**, 82,	3.3	10

45	Electronic transport in quasiperiodic decagonal aluminum. *Physical Review B*, **2001**, 65,	3.3	10
44	Stability, atomic and electronic structure of icosahedral quasicrystals. *Journal of Non-Crystalline Solids*, **1992**, 150, 337-341	3.9	10
43	Response of fcc metals and L12 and D022 type trialuminides to uniaxial loading along [100] and [001]: ab initio DFT calculations. *Philosophical Magazine*, **2011**, 91, 491-516	1.6	9
42	Catalytic properties of Al13Co4 studied by ab initio methods. *Philosophical Magazine*, **2011**, 91, 2904-2912	1.6	8
41	Magnetism at surfaces and defects in icosahedral Al-Pd-Mn quasicrystals. *Physical Review B*, **2009**, 80,	3.3	8
40	Prediction of insulating quasicrystalline approximants using ab initio electronic structure calculations. *Physical Review B*, **2003**, 67,	3.3	8
39	Theory of quasicrystal surfaces: Probing the chemical reactivity by atomic and molecular adsorption. *Surface Science*, **2008**, 602, 182-197	1.8	7
38	Ab-initio study of a quasiperiodic Bi monolayer on a fivefold icosahedral AlPdMn surface. *Philosophical Magazine*, **2006**, 86, 825-830	1.6	7
37	Electronic structure and interatomic bonding in Al10V. *Journal of Physics Condensed Matter*, **2003**, 15, 5675-5688	1.8	7
36	Fast Oxidation of Porous Cu Induced by Nano-Twinning. *Inorganic Chemistry*, **2018**, 57, 2908-2916	5.1	6
35	Bulk electronic structure of Zn-Mg-Y and Zn-Mg-Dy icosahedral quasicrystals. *Physical Review B*, **2015**, 91,	3.3	6
34	Magnetism and chemical ordering in icosahedral Al-Pd-Mn quasicrystal. *Physical Review B*, **2008**, 78,	3.3	6
33	Covalent bonding and semiconducting bandgap formation in Al-transition-metal quasicrystalline approximants. *Journal of Non-Crystalline Solids*, **2004**, 334-335, 342-346	3.9	6
32	Propagating and localized phonons in amorphous and quasicrystalline alloys. *Journal of Non-Crystalline Solids*, **1995**, 192-193, 212-221	3.9	6
31	Quasiperiodic ordering in thick Sn layer on i-Al-Pd-Mn: A possible quasicrystalline clathrate. *Physical Review Research*, **2020**, 2,	3.9	6
30	Unoccupied electronic states of icosahedral Al-Pd-Mn quasicrystals: Evidence of image potential resonance and pseudogap. *Physical Review B*, **2014**, 90,	3.3	5
29	Elementary excitations in quasicrystals. *Journal of Non-Crystalline Solids*, **1993**, 156-158, 887-890	3.9	5
28	Markov chain algorithms for canonical ensemble simulation. *Computer Physics Communications*, **1986**, 42, 29-35	4.2	5

27	Prediction of stable insulating intermetallic compounds. *Physical Review B*, **2013**, 87,	3.3	4
26	Elementary excitations in quasicrystals. *Materials Science & Engineering A: Structural Materials: Properties, Microstructure and Processing*, **1997**, 226-228, 950-960	5.3	4
25	Elementary Excitations and Physical Properties. *Springer Series in Solid-state Sciences*, **1999**, 209-256	0.4	4
24	Pair distribution function and interatomic forces in amorphous metals. *Journal of Physics F: Metal Physics*, **1984**, 14, 785-792		4
23	Structural model of quasiperiodic Pb monolayer deposited on fivefold i-Al-Pd-Mn surface. *Journal of Physics: Conference Series*, **2010**, 226, 012005	0.3	3
22	Face-centred icosahedral Al - Mg - Li alloys: a free-electron quasicrystal. *Journal of Physics Condensed Matter*, **1997**, 9, 10725-10738	1.8	3
21	Semiconductivity in aluminum□ransition-metal quasicrystalline alloys induced by ordering in six dimensions. *Europhysics Letters*, **2003**, 63, 63-68	1.6	3
20	Short-range order and the electronic structure of decagonal Al□Ni□Co. *Materials Science & Engineering A: Structural Materials: Properties, Microstructure and Processing*, **2000**, 294-296, 548-552	5.3	3
19	Ab initio study of a quasiperiodic Na monolayer on a five-fold i-Al□Pd□Mn surface. *Philosophical Magazine*, **2007**, 87, 2981-2988	1.6	2
18	Phonon localization in quasicrystals. *Journal of Non-Crystalline Solids*, **1995**, 192-193, 338-342	3.9	2
17	Atomic Structure, Interatomic Bonding and Mechanical Properties of the Al3V Compound **2005**, 289-300		2
16	Alkaline-earth metal monolayers on 5-fold i-Al□Pd□Mn surface: Influence of adatom size on quasiperiodic ordering. *Philosophical Magazine*, **2008**, 88, 2117-2122	1.6	1
15	Electronic conductivity of quasiperiodic approximants to decagonal aluminum. *Journal of Non-Crystalline Solids*, **2004**, 334-335, 363-367	3.9	1
14	Phonons and Electrons in Quasicrystals. *Springer Series in Materials Science*, **2002**, 393-420	0.9	1
13	Electronic structure of icosahedral Al?Pd?Mn alloys. *Journal of Non-Crystalline Solids*, **1995**, 192-193, 321-325	3.9	1
12	Structural and electronic properties of liquid and amorphous carbon calculated by the □fuzzy□ tight-binding Monte Carlo method. *Journal of Non-Crystalline Solids*, **1996**, 205-207, 846-850	3.9	1
11	Structure of icosahedral Al?Cu?Li(Mg) alloys: modulated tiling model. *Journal of Non-Crystalline Solids*, **1993**, 156-158, 931-935	3.9	1
10	High Catalytic Activities of RENi5□Alx (RE = La, Er) and Low Activity of Mg2Ni Following Hydrogen Uptake: The Role of Absorbed Hydrogen. *Journal of Physical Chemistry C*, **2021**, 125, 20919-20929	3.8	0

9	Origin of magnetic moments in i-AlPdMn quasicrystal. *Zeitschrift Fur Kristallographie - Crystalline Materials*, **2009**, 224, 31-34	1
8	Interatomic bonding and mechanical properties of trialuminides: an ab initio study for Al(3)(Sc,Ti,V) (abstract only). *Journal of Physics Condensed Matter*, **2008**, 20, 064222	1.8
7	Chapter 9 Ab-initio studies of quasicrystalline surfaces. *Handbook of Metal Physics*, **2008**, 3, 313-355	
6	Semiconductivity in Aluminum Transition-Metal Quasicrystals Induced by Ordering in Six Dimensions. *Ferroelectrics*, **2004**, 305, 189-192	0.6
5	Semiconducting Aluminum Transition-Metal Quasicrystals. *Materials Research Society Symposia Proceedings*, **2003**, 805, 138	
4	Ab-Initio Study of Mechanical Properties of Transition-Metal Aluminides: A Case Study for Al3(V,Ti). *Materials Science Forum*, **2005**, 482, 139-142	0.4
3	Electronic structure of hexagonal Y-Zn-Mg compound and its relation to icosahedral alloy. *Ferroelectrics*, **2001**, 250, 347-350	0.6
2	Calculation of the Electronics Structure of the (Al, Zn)-Mg Quasicrystal System. *Physica Status Solidi (B): Basic Research*, **1990**, 162, K77-K81	1.3
1	Catalytic Properties of Five-Fold Surfaces of Quasicrystal Approximants **2013**, 269-274	