Olle E Eriksson

List of Publications by Year in Descending Order

740 papers	28,032 citations	82 h-index	137 g-index
785 ext. papers	30,426 ext. citations	4.2 avg, IF	6.86 L-index

#	Paper	IF	Citations
740	Realistic first-principles calculations of the magnetocaloric effect: applications to hcp Gd. *Materials Research Letters*, **2022**, 10, 156-162	7.4	1
739	Magnon-magnon entanglement and its quantification via a microwave cavity. *Physical Review B*, **2021**, 104,	3.3	3
738	Quantifying Spin-Mixed States in Ferromagnets. *Physical Review Letters*, **2021**, 127, 207201	7.4	1
737	Alloying effect on the order-disorder transformation in tetragonal FeNi. *Scientific Reports*, **2021**, 11, 5253	4.9	2
736	Heisenberg and anisotropic exchange interactions in magnetic materials with correlated electronic structure and significant spin-orbit coupling. *Physical Review B*, **2021**, 103,	3.3	1
735	Mechanisms behind large Gilbert damping anisotropies. *Physical Review B*, **2021**, 103,	3.3	1
734	Pseudopotentials for Electronic Structure Theory. *Journal of Physical Chemistry C*, **2021**, 125, 15103-15118	3.7	1
733	Data-driven design of a new class of rare-earth free permanent magnets. *Acta Materialia*, **2021**, 212, 116913	8.4	1
732	Antichiral ferromagnetism. *Physical Review B*, **2021**, 104,	3.3	1
731	High-throughput compatible approach for entropy estimation in magnetocaloric materials: FeRh as a test case. *Journal of Alloys and Compounds*, **2021**, 857, 157811	5.7	4
730	Vibrational entropy-enhanced magnetocaloric effect in Mn-rich high-entropy alloys. *Applied Physics Letters*, **2021**, 119, 084102	3.4	3
729	Ultrafast magnetization dynamics in the half-metallic Heusler alloy Co2FeAl. *Physical Review B*, **2021**, 104,	3.3	4
728	Ab-initio study of the electronic structure and magnetic properties of Ce2Fe17. *Journal of Alloys and Compounds*, **2021**, 888, 161521	5.7	1
727	Equation of motion and the constraining field in ab initio spin dynamics. *Physical Review B*, **2020**, 102,	3.3	1
726	Self-induced spin glass state in elemental and crystalline neodymium. *Science*, **2020**, 368,	33.3	10
725	Local structure in amorphous Sm(_x)Co(_{1-x}): a combined experimental and theoretical study. *Journal of Materials Science*, **2020**, 55, 12488-12498	4.3	1
724	High-throughput and data-mining approach to predict new rare-earth free permanent magnets. *Physical Review B*, **2020**, 101,	3.3	14

723	Localized versus itinerant character of 4f-states in cerium oxides. *Journal of Physics Condensed Matter*, **2020**, 32, 215502	1.8	2
722	Nonreciprocal spin pumping damping in asymmetric magnetic trilayers. *Physical Review B*, **2020**, 101,	3.3	4
721	Direct writing of lateral fluorographene nanopatterns with tunable bandgaps and its application in new generation of moir superlattice. *Applied Physics Reviews*, **2020**, 7, 011403	17.3	11
720	Direct light-induced spin transfer between different elements in a spintronic Heusler material via femtosecond laser excitation. *Science Advances*, **2020**, 6, eaaz1100	14.3	22
719	Magnetic two-dimensional electron liquid at the surface of Heusler semiconductors. *Physical Review Materials*, **2020**, 4,	3.2	2
718	Analysis of the linear relationship between asymmetry and magnetic moment at the M edge of 3d transition metals. *Physical Review Research*, **2020**, 2,	3.9	10
717	Localized surface electromagnetic waves in CrI-based magnetophotonic structures. *Optics Express*, **2020**, 28, 29155-29165	3.3	1
716	Theoretical Methods. *SpringerBriefs in Applied Sciences and Technology*, **2020**, 19-24	0.4	
715	Multiscale approach for magnetization dynamics: unraveling exotic magnetic states of matter. *Physical Review Research*, **2020**, 2,	3.9	1
714	Electron Correlation and Spin Transition. *SpringerBriefs in Applied Sciences and Technology*, **2020**, 35-43	0.4	
713	Hierarchy of magnon mode entanglement in antiferromagnets. *Physical Review B*, **2020**, 102,	3.3	3
712	Electronic Structure of Isolated Molecules. *SpringerBriefs in Applied Sciences and Technology*, **2020**, 25-34	0.4	1
711	Interaction with Substrates. *SpringerBriefs in Applied Sciences and Technology*, **2020**, 45-64	0.4	1
710	Soft X-Ray Magnetic Circular Dichroism of Vanadium in the Metal Insulator Two-Phase Region of Paramagnetic V2O3 Doped with 1.1% Chromium. *Physica Status Solidi (B): Basic Research*, **2020**, 257, 1900456	1.3	0
709	Measuring the Intra-Atomic Exchange Energy in Rare-Earth Adatoms. *Physical Review X*, **2020**, 10,	9.1	3
708	Partial cation ordering, relaxor ferroelectricity, and ferrimagnetism in Pb(Fe1 xYbx)2/3W1/3O3 solid solutions. *Journal of Applied Physics*, **2020**, 128, 134102	2.5	
707	Interlayer charge transfer in tin disulphide: Orbital anisotropy and temporal aspects. *Physical Review B*, **2020**, 102,	3.3	3
706	Coexistence of Superconductivity and Charge Density Waves in Tantalum Disulfide: Experiment and Theory. *Physical Review Letters*, **2020**, 125, 186401	7.4	7

705	Pressure effect on the order-disorder transformation in L1 FeNi. *Scientific Reports*, **2020**, 10, 14766	4.9	2
704	First-principles Dzyaloshinskii-Moriya interaction in a non-collinear framework. *Scientific Reports*, **2020**, 10, 20339	4.9	4
703	Photoelectron Spectroscopy of Molecules Beyond the Electric Dipole Approximation. *Journal of Chemical Theory and Computation*, **2019**, 15, 5483-5494	6.4	3
702	Atomic photoionization cross sections beyond the electric dipole approximation. *Journal of Chemical Physics*, **2019**, 150, 044306	3.9	4
701	Database of novel magnetic materials for high-performance permanent magnet development. *Computational Materials Science*, **2019**, 168, 188-202	3.2	21
700	Density Functional Theory description of the order-disorder transformation in Fe-Ni. *Scientific Reports*, **2019**, 9, 8172	4.9	7
699	Ligand Effects on the Linear Response Hubbard U: The Case of Transition Metal Phthalocyanines. *Journal of Physical Chemistry A*, **2019**, 123, 3214-3222	2.8	5
698	General method for atomistic spin-lattice dynamics with first-principles accuracy. *Physical Review B*, **2019**, 99,	3.3	13
697	Charge disproportionate antiferromagnetism at the verge of the insulator-metal transition in doped LaFeO3. *Physical Review B*, **2019**, 99,	3.3	9
696	Europium Cyclooctatetraene Nanowire Carpets: A Low-Dimensional, Organometallic, and Ferromagnetic Insulator. *Journal of Physical Chemistry Letters*, **2019**, 10, 911-917	6.4	7
695	Plastic deformation transition in FeCrCoNiAlx high-entropy alloys. *Materials Research Letters*, **2019**, 7, 439-445	7.4	9
694	Cation ordering, ferrimagnetism and ferroelectric relaxor behavior in Pb(Fe1−xScx)2−W1−O3 solid solutions. *European Physical Journal B*, **2019**, 92, 1	1.2	4
693	Peculiar magnetic states in the double perovskite Nd2NiMnO6. *Physical Review B*, **2019**, 100,	3.3	5
692	Electronic specific heat coefficient and magnetic properties of Y(Fe1−Cox)2 Laves phases: A combined experimental and first-principles study. *Physical Review B*, **2019**, 100,	3.3	1
691	Spin polaronics: Static and dynamic properties of spin polarons in La-doped CaMnO3. *Physical Review B*, **2019**, 100,	3.3	3
690	Influence of antiphase boundary of the MnAl −phase on the energy product. *Physical Review Materials*, **2019**, 3,	3.2	1
689	Self-organizing maps as a method for detecting phase transitions and phase identification. *Physical Review B*, **2019**, 99,	3.3	11
688	Suppression of the Verwey Transition by Charge Trapping. *Annalen Der Physik*, **2018**, 530, 1700363	2.6	6

687	Searching for materials with reduced dimension. *Nature Nanotechnology*, **2018**, 13, 180-181	28.7	6
686	Mapping the magnetic transition temperatures for medium- and high-entropy alloys. *Intermetallics*, **2018**, 95, 80-84	3.5	50
685	Investigation of the spectral properties and magnetism of BiFeO3 by dynamical mean-field theory. *Physical Review B*, **2018**, 97,	3.3	6
684	Coupling atomistic and continuum modelling of magnetism. *Computer Methods in Applied Mechanics and Engineering*, **2018**, 329, 219-253	5.7	7
683	Magnetic anisotropy in permalloy: Hidden quantum mechanical features. *Physical Review B*, **2018**, 97,	3.3	6
682	A majority gate with chiral magnetic solitons. *Journal of Physics Condensed Matter*, **2018**, 30, 375801	1.8	6
681	Nonlocal Gilbert damping tensor within the torque-torque correlation model. *Physical Review Materials*, **2018**, 2,	3.2	10
680	Heavy-mass magnetic modes in pyrochlore iridates due to dominant Dzyaloshinskii-Moriya interaction. *Physical Review Materials*, **2018**, 2,	3.2	13
679	Hexagonal M2C3 (M = As, Sb, and Bi) monolayers: new functional materials with desirable band gaps and ultrahigh carrier mobility. *Journal of Materials Chemistry C*, **2018**, 6, 12689-12697	7.1	30
678	First-principles calculations of the ultralow thermal conductivity in two-dimensional group-IV selenides. *Physical Review B*, **2018**, 98,	3.3	48
677	Another view on Gilbert damping in two-dimensional ferromagnets. *Scientific Reports*, **2018**, 8, 17148	4.9	3
676	On the origin of perpendicular magnetic anisotropy in strained Fe□o(□) films. *Journal Physics D: Applied Physics*, **2017**, 50, 045003	3	4
675	Enhanced spin-orbit coupling in tetragonally strained Fe-Co-B films. *Journal of Physics Condensed Matter*, **2017**, 29, 275802	1.8	10
674	Exchange interactions of CaMnO3 in the bulk and at the surface. *Physical Review B*, **2017**, 95,	3.3	13
673	AlMB (M = Cr, Mn, Fe, Co, Ni): a group of nanolaminated materials. *Journal of Physics Condensed Matter*, **2017**, 29, 155402	1.8	44
672	Evolution of the structural and multiferroic properties of PbFe2/3W1/3O3 ceramics upon Mn-doping. *Materials Chemistry and Physics*, **2017**, 187, 218-232	4.4	6
671	Theory of noncollinear interactions beyond Heisenberg exchange: Applications to bcc Fe. *Physical Review B*, **2017**, 96,	3.3	10
670	Magnetic properties of the Fe5SiB2□e5PB2 system. *Physical Review B*, **2017**, 96,	3.3	8

669	Prediction of the new efficient permanent magnet SmCoNiFe3. *Physical Review B*, **2017**, 96,	3.3	28
668	Spin-polaron formation and magnetic state diagram in La-doped CaMnO3. *Physical Review B*, **2017**, 95,	3.3	5
667	Towards sub-nanometer real-space observation of spin and orbital magnetism at the Fe/MgO interface. *Scientific Reports*, **2017**, 7, 44802	4.9	12
666	The Bethe-Slater curve revisited; new insights from electronic structure theory. *Scientific Reports*, **2017**, 7, 4058	4.9	20
665	Topological edge-state engineering with high-frequency electromagnetic radiation. *Physical Review B*, **2017**, 96,	3.3	6
664	Magnetism and ultrafast magnetization dynamics of Co and CoMn alloys at finite temperature. *Physical Review B*, **2017**, 95,	3.3	10
663	First-principles theory of electronic structure and magnetism of Cr nano-islands on Pd(1 1 1). *Journal of Physics Condensed Matter*, **2017**, 29, 025807	1.8	0
662	Structural, electronic, and thermodynamic properties of curium dioxide: Density functional theory calculations. *Physical Review B*, **2017**, 96,	3.3	22
661	Theory of L-edge spectroscopy of strongly correlated systems. *Physical Review B*, **2017**, 96,	3.3	13
660	Combining electronic structure and many-body theory with large databases: A method for predicting the nature of 4f states in Ce compounds. *Physical Review Materials*, **2017**, 1,	3.2	9
659	Atomistic Spin Dynamics **2017**,		67
658	Electronic structure and exchange interactions of insulating double perovskite La2CuRuO6. *Physical Review B*, **2016**, 94,	3.3	7
657	Standard model of the rare earths analyzed from the Hubbard I approximation. *Physical Review B*, **2016**, 94,	3.3	45
656	Finite-temperature interatomic exchange and magnon softening in Fe overlayers on Ir(001). *Physical Review B*, **2016**, 94,	3.3	6
655	Analytic continuation by averaging Pad approximants. *Physical Review B*, **2016**, 93,	3.3	26
654	Electronic and magnetic properties of single Fe atoms on a CuN surface: Effects of electron correlations. *Physical Review B*, **2016**, 93,	3.3	12
653	Correlated electron behavior of metal-organic molecules: Insights from density functional theory combined with many-body effects using exact diagonalization. *Physical Review B*, **2016**, 93,	3.3	13
652	First-principles studies of the Gilbert damping and exchange interactions for half-metallic Heuslers alloys. *Physical Review B*, **2016**, 93,	3.3	16

651	Correlation effects and orbital magnetism of Co clusters. *Physical Review B*, **2016**, 93,	3.3	11
650	High photon energy spectroscopy of NiO: Experiment and theory. *Physical Review B*, **2016**, 93,	3.3	15
649	First-principles investigation of two-dimensional trichalcogenide and sesquichalcogenide monolayers. *Physical Review B*, **2016**, 93,	3.3	26
648	Microscopic Origin of Heisenberg and Non-Heisenberg Exchange Interactions in Ferromagnetic bcc Fe. *Physical Review Letters*, **2016**, 116, 217202	7.4	48
647	Magnetic properties of Fe5SiB2 and its alloys with P, S, and Co. *Physical Review B*, **2016**, 93,	3.3	14
646	A spin dynamics approach to solitonics. *Scientific Reports*, **2016**, 6, 25685	4.9	13
645	Reproducibility in density functional theory calculations of solids. *Science*, **2016**, 351, aad3000	33.3	784
644	Low temperature magneto-structural transitions in Mn3Ni20P6. *Journal of Solid State Chemistry*, **2016**, 237, 343-348	3.3	2
643	Magnetic and electronic structure of Mn nanostructures on Ag(111) and Au(111). *Physical Review B*, **2016**, 93,	3.3	10
642	Influence of Electron Correlation on the Electronic Structure and Magnetism of Transition-Metal Phthalocyanines. *Journal of Chemical Theory and Computation*, **2016**, 12, 1772-85	6.4	45
641	Mapping of Defects in Individual Silicon Nanocrystals Using Real-Space Spectroscopy. *Journal of Physical Chemistry Letters*, **2016**, 7, 1047-54	6.4	8
640	Polar Order and Frustrated Antiferromagnetism in Perovskite Pb2MnWO6 Single Crystals. *Inorganic Chemistry*, **2016**, 55, 2791-805	5.1	16
639	Correlated electronic structure of CeN. *Journal of Electron Spectroscopy and Related Phenomena*, **2016**, 208, 111-115	1.7	1
638	Women with Premenstrual Dysphoria Lack the Seemingly Normal Premenstrual Right-Sided Relative Dominance of 5-HTP-Derived Serotonergic Activity in the Dorsolateral Prefrontal Cortices - A Possible Cause of Disabling Mood Symptoms. *PLoS ONE*, **2016**, 11, e0159538	3.7	7
637	Ab initio investigation of competing antiferromagnetic structures in low Si-content FeMn(PSi) alloy. *Journal of Physics Condensed Matter*, **2016**, 28, 216002	1.8	2
636	Many-body effects and excitonic features in 2D biphenylene carbon. *Journal of Chemical Physics*, **2016**, 144, 024702	3.9	10
635	Magnetism and exchange interaction of small rare-earth clusters; Tb as a representative. *Scientific Reports*, **2016**, 6, 19676	4.9	18
634	Site-selective local fluorination of graphene induced by focused ion beam irradiation. *Scientific Reports*, **2016**, 6, 19719	4.9	30

633	Scale Transitions in Magnetisation Dynamics. *Communications in Computational Physics*, **2016**, 20, 969-988	2.4	6
632	Communication: Visualization and spectroscopy of defects induced by dehydrogenation in individual silicon nanocrystals. *Journal of Chemical Physics*, **2016**, 144, 241102	3.9	2
631	Ultra-low magnetic damping of a metallic ferromagnet. *Nature Physics*, **2016**, 12, 839-842	16.2	199
630	A new 2D monolayer BiXene, M2C (M = Mo, Tc, Os). *Nanoscale*, **2016**, 8, 15753-62	7.7	35
629	Valence and spectral properties of rare-earth clusters. *Physical Review B*, **2015**, 92,	3.3	9
628	First-principles study of the influence of different interfaces and core types on the properties of CdSe/CdS core-shell nanocrystals. *Scientific Reports*, **2015**, 5, 10865	4.9	18
627	Two-Dimensional Indium Selenides Compounds: An Ab Initio Study. *Journal of Physical Chemistry Letters*, **2015**, 6, 3098-103	6.4	156
626	Toward Rare-Earth-Free Permanent Magnets: A Combinatorial Approach Exploiting the Possibilities of Modeling, Shape Anisotropy in Elongated Nanoparticles, and Combinatorial Thin-Film Approach. *Jom*, **2015**, 67, 1318-1328	2.1	29
625	Size dependence of the stability, electronic structure, and optical properties of silicon nanocrystals with various surface impurities. *Physical Review B*, **2015**, 91,	3.3	10
624	The electronic characterization of biphenylene--experimental and theoretical insights from core and valence level spectroscopy. *Journal of Chemical Physics*, **2015**, 142, 074305	3.9	19
623	Lattice dynamics and chemical bonding in Sb2Te3 from first-principles calculations. *Journal of Chemical Physics*, **2015**, 142, 174702	3.9	19
622	Controlling Electronic Structure and Transport Properties of Zigzag Graphene Nanoribbons by Edge Functionalization with Fluorine. *Journal of Physical Chemistry C*, **2015**, 119, 21227-21233	3.8	15
621	Atomic contributions to the valence band photoelectron spectra of metal-free, iron and manganese phthalocyanines. *Journal of Electron Spectroscopy and Related Phenomena*, **2015**, 205, 92-97	1.7	7
620	Magnetic properties of (Fe1−xCox)2B alloys and the effect of doping by 5d elements. *Physical Review B*, **2015**, 92,	3.3	48
619	Quasi-2D Cu2 S crystals on graphene: in-situ growth and ab-initio calculations. *Small*, **2015**, 11, 1253-7	11	20
618	Amorphous WSN thin films: The atomic structure behind ultra-low friction. *Acta Materialia*, **2015**, 82, 84-93	8.4	28
617	Dynamic Stabilization of Cubic AuZn. *Materials Today: Proceedings*, **2015**, 2, S569-S572	1.4	
616	Exchange parameters of strongly correlated materials: Extraction from spin-polarized density functional theory plus dynamical mean-field theory. *Physical Review B*, **2015**, 91,	3.3	64

615	All-thermal switching of amorphous Gd-Fe alloys: Analysis of structural properties and magnetization dynamics. *Physical Review B*, **2015**, 92,	3.3	32
614	Gilbert-like damping caused by time retardation in atomistic magnetization dynamics. *Physical Review B*, **2015**, 92,	3.3	9
613	Polaron mobility in oxygen-deficient and lithium-doped tungsten trioxide. *Physical Review B*, **2015**, 92,	3.3	43
612	Layer-resolved magnetic exchange interactions of surfaces of late 3d elements: Effects of electronic correlations. *Physical Review B*, **2015**, 92,	3.3	9
611	Monovacancy formation energies and Fermi surface topological transitions in Pd-Ag alloys. *Physical Review B*, **2015**, 92,	3.3	4
610	Influence of dimensionality and interface type on optical and electronic properties of CdS/ZnS core-shell nanocrystals--A first-principles study. *Journal of Chemical Physics*, **2015**, 143, 164701	3.9	7
609	Thermodynamic-state and kinetic-process dependent dual ferromagnetic states in high-Si content FeMn(PSi) alloys. *Journal of Applied Physics*, **2015**, 118, 213903	2.5	5
608	Effect of uniaxial strain on the site occupancy of hydrogen in vanadium from density-functional calculations. *Scientific Reports*, **2015**, 5, 10301	4.9	14
607	Large-eddy simulations of wind farm production and long distance wakes. *Journal of Physics: Conference Series*, **2015**, 625, 012022	0.3	
606	Wake downstream of the Lillgrund wind farm - A Comparison between LES using the actuator disc method and a Wind farm Parametrization in WRF. *Journal of Physics: Conference Series*, **2015**, 625, 012028	0.3	19
605	Dynamics of quasiparticles in graphene under intense circularly polarized light. *Physical Review B*, **2015**, 91,	3.3	17
604	Atomistic spin dynamics and surface magnons. *Journal of Physics Condensed Matter*, **2015**, 27, 243202	1.8	12
603	Electronic topological transition and noncollinear magnetism in compressed hcp Co. *Physical Review B*, **2015**, 92,	3.3	16
602	The influence of oxygen adsorption on the NEXAFS and core-level XPS spectra of the C60 derivative PCBM. *Journal of Chemical Physics*, **2015**, 142, 054306	3.9	18
601	Laser Heated Ferromagnetic Simulations. *Springer Proceedings in Physics*, **2015**, 76-78	0.2	
600	Coarse-Graining Approach to Atomistic Spin Dynamics. *Springer Proceedings in Physics*, **2015**, 162-165	0.2	
599	The dipole moment of the spin density as a local indicator for phase transitions. *Scientific Reports*, **2014**, 4, 5760	4.9	17
598	Lattice dynamics of cubic AuZn from first principles. *Physical Review B*, **2014**, 89,	3.3	2

597	Field-regulated switching of the magnetization of Co-porphyrin on graphene. *Physical Review B*, **2014**, 89,	3.3	14
596	Elucidating the 3d electronic configuration in manganese phthalocyanine. *Journal of Physical Chemistry A*, **2014**, 118, 927-32	2.8	40
595	Anisotropy of magnetic properties of Fe(1+y)Te. *Journal of Physics Condensed Matter*, **2014**, 26, 436003	1.8	2
594	Electronic structure, cohesive properties, and magnetism of SrRuO3. *Physical Review B*, **2014**, 90,	3.3	15
593	Tuning order-by-disorder multiferroicity in CuO by doping. *Physical Review B*, **2014**, 90,	3.3	13
592	Thermally driven domain-wall motion in Fe on W(110). *Physical Review B*, **2014**, 90,	3.3	21
591	Hole bipolaron formation at (100) MgO/CaO epitaxial interface. *Physical Review B*, **2014**, 89,	3.3	7
590	Fermi condensation near van Hove singularities within the Hubbard model on the triangular lattice. *Physical Review Letters*, **2014**, 112, 070403	7.4	84
589	Electronic structure of In3Se4 and In3Te4 monolayers from ab-initio calculations. *Annalen Der Physik*, **2014**, 526, 402-407	2.6	4
588	Stabilization of the tetragonal distortion of FexCo1 alloys by C impurities: A potential new permanent magnet. *Physical Review B*, **2014**, 89,	3.3	46
587	Topological excitations in a kagome magnet. *Nature Communications*, **2014**, 5, 4815	17.4	57
586	Electronic structure of two-dimensional transition metal dichalcogenide bilayers from ab initio theory. *Physical Review B*, **2014**, 89,	3.3	88
585	Effect of spin orbit coupling and Hubbard U on the electronic structure of IrO2. *Physical Review B*, **2014**, 89,	3.3	29
584	Analysis of long distance wakes of Horns Rev I using actuator disc approach. *Journal of Physics: Conference Series*, **2014**, 555, 012032	0.3	3
583	Analysis of long distance wakes behind a row of turbines a parameter study. *Journal of Physics: Conference Series*, **2014**, 524, 012152	0.3	3
582	Formation of 2D transition metal dichalcogenides on TiC1Ax surfaces (A = S, Se, Te): A theoretical study. *Journal of Materials Research*, **2014**, 29, 207-214	2.5	2
581	Kinetic arrest induced antiferromagnetic order in hexagonal FeMnP0.75Si0.25 alloy. *Applied Physics Letters*, **2014**, 105, 262405	3.4	10
580	Comparison of van der Waals corrected and sparse-matter density functionals for the metal-free phthalocyanine/gold interface. *Physical Review B*, **2014**, 89,	3.3	33

579	Fen (n=1–8) clusters chemisorbed on vacancy defects in graphene: Stability, spin-dipole moment, and magnetic anisotropy. *Physical Review B*, **2014**, 89,	3.3	15
578	Microscopic description of the evolution of the local structure and an evaluation of the chemical pressure concept in a solid solution. *Physical Review B*, **2014**, 89,	3.3	17
577	Origin of the magnetostructural coupling in FeMnP0.75Si0.25. *Physical Review B*, **2014**, 90,	3.3	14
576	Fe phthalocyanine on Co(001): Influence of surface oxidation on structural and electronic properties. *Physical Review B*, **2014**, 89,	3.3	17
575	Treatment of 4f states of the rare earths: The case study of TbN. *Physical Review B*, **2014**, 89,	3.3	20
574	Revisiting the adsorption of copper-phthalocyanine on Au(111) including van der Waals corrections. *Journal of Chemical Physics*, **2014**, 140, 124711	3.9	10
573	Magnetic properties of Fe(x)Co(1-x) nanochains on Pt(1 1 1) surfaces. *Journal of Physics Condensed Matter*, **2014**, 26, 206003	1.8	2
572	A charge self-consistent LDA+DMFT study of the spectral properties of hexagonal NiS. *New Journal of Physics*, **2014**, 16, 093049	2.9	1
571	Two-Dimensional Materials from Data Filtering and Ab Initio Calculations. *Physical Review X*, **2013**, 3,	9.1	141
570	X-ray absorption spectra: Graphene, h-BN, and their alloy. *Physical Review B*, **2013**, 87,	3.3	5
569	Identifying the electronic character and role of the Mn states in the valence band of (Ga,Mn)As. *Physical Review Letters*, **2013**, 111, 097201	7.4	27
568	Iron porphyrin molecules on Cu(001): Influence of adlayers and ligands on the magnetic properties. *Physical Review B*, **2013**, 87,	3.3	27
567	Electronic structure and magnetic properties of Mn, Co, and Ni substitution of Fe in Fe4N. *Physical Review B*, **2013**, 88,	3.3	25
566	Transition between direct and indirect band gap in silicon nanocrystals. *Physical Review B*, **2013**, 87,	3.3	36
565	Interatomic exchange interactions for finite-temperature magnetism and nonequilibrium spin dynamics. *Physical Review Letters*, **2013**, 111, 127204	7.4	60
564	Designing Fe Nanostructures at Graphene/h-BN Interfaces. *Journal of Physical Chemistry C*, **2013**, 117, 21763-21771	3.8	7
563	Effects of strain on ferroelectric polarization and magnetism in orthorhombic HoMnO3. *Physical Review B*, **2013**, 87,	3.3	15
562	Hydrogen storage properties of the pseudo binary laves phase (Sc1−xZrx)(Co1−yNiy)2 system. *International Journal of Hydrogen Energy*, **2013**, 38, 9772-9778	6.7	4

561	Correlated electronic structure of Fe in bulk Cs and on a Cs surface. *Physical Review B*, **2013**, 87,	3.3	1
560	Possible high-temperature superconductors predicted from electronic structure and data-filtering algorithms. *Computational Materials Science*, **2013**, 67, 282-286	3.2	20
559	Photoelectron and Absorption Spectroscopy Studies of Metal-Free Phthalocyanine on Au(111): Experiment and Theory. *Journal of Physical Chemistry C*, **2013**, 117, 7018-7025	3.8	15
558	Defect controlled magnetism in FeP/graphene/Ni(111). *Scientific Reports*, **2013**, 3, 3405	4.9	28
557	Electron correlations in Mn(x)Ga(1-x)A(s)as seen by resonant electron spectroscopy and dynamical mean field theory. *Nature Communications*, **2013**, 4, 2645	17.4	38
556	Phonon spectrum, thermodynamic properties, and pressure-temperature phase diagram of uranium dioxide. *Physical Review B*, **2013**, 88,	3.3	57
555	Atomistic spin dynamics of low-dimensional magnets. *Physical Review B*, **2013**, 87,	3.3	44
554	Oxygen-tuned magnetic coupling of Fe-phthalocyanine molecules to ferromagnetic Co films. *Physical Review B*, **2013**, 88,	3.3	32
553	Manipulation of spin state of iron porphyrin by chemisorption on magnetic substrates. *Physical Review B*, **2013**, 88,	3.3	40
552	Experimental and theoretical study of electronic structure of lutetium bi-phthalocyanine. *Journal of Chemical Physics*, **2013**, 138, 234701	3.9	13
551	Tribochemically Active TiCS Nanocomposite Coatings. *Materials Research Letters*, **2013**, 1, 148-155	7.4	8
550	Nanosession: Multiferroics - High Transition Temperatures **2013**, 347-355		
549	Complex magnetic structure of clusters and chains of Ni and Fe on Pt(111). *Scientific Reports*, **2013**, 3, 3054	4.9	18
548	Ovarian morphology in premenstrual dysphoria. *Psychoneuroendocrinology*, **2012**, 37, 742-51	5	4
547	Theory of diluted magnetic semiconductors. *Science and Technology of Atomic, Molecular, Condensed Matter and Biological Systems*, **2012**, 2, 1-19		1
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