Olle E Eriksson

List of Publications by Citations

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	Density functional theory for calculation of elastic properties of orthorhombic crystals: Application to TiSi2. *Journal of Applied Physics*, **1998**, 84, 4891-4904	2.5	1239
739	First-principles theory of dilute magnetic semiconductors. *Reviews of Modern Physics*, **2010**, 82, 1633-1690	40.5	855
738	Electronic structure of two-dimensional crystals from ab initio theory. *Physical Review B*, **2009**, 79,	3.3	851
737	Reproducibility in density functional theory calculations of solids. *Science*, **2016**, 351, aad3000	33.3	784
736	Theoretical investigation of magnetoelectric behavior in BiFeO3. *Physical Review B*, **2006**, 74,	3.3	501
735	Elastic constants of hexagonal transition metals: Theory. *Physical Review B*, **1995**, 51, 17431-17438	3.3	501
734	Substrate-induced magnetic ordering and switching of iron porphyrin molecules. *Nature Materials*, **2007**, 6, 516-20	27	360
733	Orbital polarization in narrow-band systems: Application to volume collapses in light lanthanides. *Physical Review B*, **1990**, 41, 7311-7314	3.3	301
732	Giant magnetic anisotropy in tetragonal FeCo alloys. *Physical Review Letters*, **2004**, 93, 027203	7.4	284
731	Entropy driven stabilization of energetically unstable crystal structures explained from first principles theory. *Physical Review Letters*, **2008**, 100, 095901	7.4	260
730	Accurate electronic band gap of pure and functionalized graphane from GW calculations. *Physical Review B*, **2009**, 79,	3.3	256
729	Magnetic percolation in diluted magnetic semiconductors. *Physical Review Letters*, **2004**, 93, 137202	7.4	250
728	Structural, elastic, and high-pressure properties of cubic TiC, TiN, and TiO. *Physical Review B*, **1996**, 53, 3072-3079	3.3	243
727	Orbital magnetism in Fe, Co, and Ni. *Physical Review B*, **1990**, 42, 2707-2710	3.3	226
726	Theory of elastic constants of cubic transition metals and alloys. *Physical Review B*, **1993**, 48, 5844-5851	3.3	214
725	Enhancement of Orbital Magnetism at Surfaces: Co on Cu(100). *Physical Review Letters*, **1995**, 75, 1602-1605	7.4	200
724	Ultra-low magnetic damping of a metallic ferromagnet. *Nature Physics*, **2016**, 12, 839-842	16.2	199

723	Mn+1AXn phases in the Ti-Si-C system studied by thin-film synthesis and ab initio calculations. *Physical Review B*, **2004**, 70,	3.3	188
722	4f-band magnetism in CeFe2. *Physical Review Letters*, **1988**, 60, 2523-2526	7.4	188
721	Deposition and characterization of ternary thin films within the Ti-Al-C system by DC magnetron sputtering. *Journal of Crystal Growth*, **2006**, 291, 290-300	1.6	187
720	A method for atomistic spin dynamics simulations: implementation and examples. *Journal of Physics Condensed Matter*, **2008**, 20, 315203	1.8	184
719	Ultrafast spin dynamics in multisublattice magnets. *Physical Review Letters*, **2012**, 108, 057202	7.4	178
718	Tailoring the nature of magnetic coupling of Fe-porphyrin molecules to ferromagnetic substrates. *Physical Review Letters*, **2009**, 102, 047202	7.4	173
717	A unified picture of the crystal structures of metals. *Nature*, **1995**, 374, 524-525	50.4	172
716	Total energy calculation of the magnetocrystalline anisotropy energy in the ferromagnetic 3d metals. *Physical Review Letters*, **1995**, 75, 2871-2874	7.4	169
715	Large magnetocrystalline anisotropy in bilayer transition metal phases from first-principles full-potential calculations. *Physical Review B*, **2001**, 63,	3.3	163
714	Calculated spin and orbital moments in the surfaces of the 3d metals Fe, Co, and Ni and their overlayers on Cu(001). *Physical Review B*, **1996**, 53, 9204-9213	3.3	159
713	Experimental and theoretical identification of a new high-pressure phase of silica. *Nature*, **1997**, 388, 362-365	50.4	158
712	Two-Dimensional Indium Selenides Compounds: An Ab Initio Study. *Journal of Physical Chemistry Letters*, **2015**, 6, 3098-103	6.4	156
711	Full-potential optical calculations of lead chalcogenides. *International Journal of Quantum Chemistry*, **1998**, 69, 349-358	2.1	154
710	Two-Dimensional Materials from Data Filtering and Ab Initio Calculations. *Physical Review X*, **2013**, 3,	9.1	141
709	Crystal structures of Ti, Zr, and Hf under compression: Theory. *Physical Review B*, **1993**, 48, 16269-16279	3.3	139
708	Molecular adsorption in graphene with divacancy defects. *Physical Review B*, **2009**, 79,	3.3	136
707	Calculated magnetic properties of binary alloys between Fe, Co, Ni, and Cu. *Physical Review B*, **1999**, 59, 419-430	3.3	136
706	Electronic structure, chemical bonding, and optical properties of ferroelectric and antiferroelectric NaNO2. *Physical Review B*, **1999**, 59, 1776-1785	3.3	136

705	Magnetic anisotropy and magnetostriction in tetragonal and cubic Ni. *Physical Review B*, **1997**, 55, 15026-15032	3.3	132
704	3d-5d band magnetism in rare earth transition metal intermetallics: LuFe2. *Journal of Physics Condensed Matter*, **1989**, 1, 5861-5874	1.8	129
703	Theory of bulk and surface quasiparticle spectra for Fe, Co, and Ni. *Physical Review B*, **2007**, 76,	3.3	126
702	Prediction of ferromagnetism and metamagnetism in 4d transition-metal overlayers on the (001) surface of Ag (4d=Tc, Ru, Rh, and Pd). *Physical Review Letters*, **1991**, 66, 1350-1353	7.4	126
701	Positron emission tomography in clinical islet transplantation. *American Journal of Transplantation*, **2009**, 9, 2816-24	8.7	125
700	Electronic properties of f-electron metals using the generalized gradient approximation. *Physical Review B*, **1994**, 50, 7291-7294	3.3	125
699	Spin and orbital magnetism in Fe-Co and Co-Ni alloys. *Physical Review B*, **1992**, 45, 12911-12916	3.3	125
698	Optical properties of the group-IVB refractory metal compounds. *Physical Review B*, **1996**, 54, 1673-1681	3.3	124
697	Ferromagnetic materials in the zinc-blende structure. *Physical Review B*, **2003**, 68,	3.3	123
696	Novel electronic configuration in □u. *Journal of Alloys and Compounds*, **1999**, 287, 1-5	5.7	121
695	Theoretical analysis of the chemical bonding and electronic structure of graphene interacting with Group IA and Group VIIA elements. *Physical Review B*, **2010**, 81,	3.3	120
694	Analysis of reproducibility of subjective grading systems for breast carcinoma. *Journal of Clinical Pathology*, **1979**, 32, 979-85	3.9	118
693	Phase stabilities and structural relaxations in substoichiometric TiC1□. *Physical Review B*, **2001**, 63,	3.3	117
692	Magnetic, optical, and magneto-optical properties of MnX (X=As, Sb, or Bi) from full-potential calculations. *Physical Review B*, **1999**, 59, 15680-15693	3.3	115
691	Perpendicular magnetocrystalline anisotropy in tetragonally distorted Fe-Co alloys. *Physical Review Letters*, **2006**, 96, 037205	7.4	112
690	Theoretical aspects of the FecNi1-c Invar alloy. *Physical Review B*, **1995**, 51, 1058-1063	3.3	112
689	Data mining and accelerated electronic structure theory as a tool in the search for new functional materials. *Computational Materials Science*, **2009**, 44, 1042-1049	3.2	108
688	Optical properties of graphite from first-principles calculations. *Physical Review B*, **1997**, 55, 4999-5005	3.3	108

687	Pharmacokinetics of tranexamic acid after intravenous administration to normal volunteers. *European Journal of Clinical Pharmacology*, **1974**, 7, 375-80	2.8	108
686	Full-Potential Electronic Structure Method. *Springer Series in Solid-state Sciences*, **2010**,	0.4	106
685	Formation and structure of graphene waves on Fe(110). *Physical Review Letters*, **2012**, 109, 026101	7.4	105
684	Defect formation in graphene nanosheets by acid treatment: an x-ray absorption spectroscopy and density functional theory study. *Journal Physics D: Applied Physics*, **2008**, 41, 062001	3	105
683	Crystal-structure stabilities and electronic structure for the light actinides Th, Pa, and U. *Physical Review B*, **1992**, 45, 13879-13890	3.3	105
682	Defect-induced magnetic structure in (Ga(1)-(x)Mn(x))As. *Physical Review Letters*, **2002**, 88, 187202	7.4	104
681	Ground-state and excited-state properties of LaMnO3 from full-potential calculations. *Physical Review B*, **2002**, 65,	3.3	103
680	Crystal structure and elastic-constant anomalies in the magnetic 3d transition metals. *Physical Review B*, **1994**, 50, 5918-5927	3.3	103
679	Influence of ligand states on the relationship between orbital moment and magnetocrystalline anisotropy. *Physical Review Letters*, **2007**, 99, 177207	7.4	102
678	Cardiac glycosides and breast cancer. *Lancet, The*, **1979**, 1, 563	40	100
677	Adsorption of Cu, Ag, and Au atoms on graphene including van der Waals interactions. *Journal of Physics Condensed Matter*, **2011**, 23, 395001	1.8	99
676	Magnetic anisotropy of L10 FePt and Fe1□MnxPt. *Physical Review B*, **2005**, 71,	3.3	99
675	Quasi ab initio molecular dynamic study of Cu melting. *Physical Review B*, **2000**, 61, 3838-3844	3.3	99
674	Effects of growth hormone substitution on mental performance in adults with growth hormone deficiency: a pilot study. *Psychoneuroendocrinology*, **1986**, 11, 347-52	5	98
673	Surface energies and work functions of the transition metal carbides. *Surface Science*, **2004**, 557, 243-254	1.8	97
672	Meta-magnetism in UCoAl. *Journal of Physics Condensed Matter*, **1989**, 1, 4005-4011	1.8	97
671	Theoretical aspects of the magnetism in the ferromagnetic AFe2 systems (A=U, Np, Pu, and Am). *Physical Review B*, **1990**, 41, 9087-9094	3.3	96
670	Strength of correlation effects in the electronic structure of iron. *Physical Review Letters*, **2009**, 103, 267203	7.4	95

669	Theoretical study of the magnetism of Mn-doped ZnO with and without defects. *Physical Review B*, **2006**, 74,	3.3	94
668	Trends of the elastic constants of cubic transition metals. *Physical Review Letters*, **1992**, 68, 2802-2805	7.4	93
667	Restricting dislocation movement in transition metal carbides by phase stability tuning. *Science*, **2001**, 293, 2434-7	33.3	92
666	Theory of ferromagnetism in CeCo5. *Physical Review B*, **1990**, 41, 9111-9120	3.3	92
665	Structural properties of plutonium from first-principles theory. *Physical Review B*, **1997**, 55, 1997-2004	3.3	90
664	Elastic and high pressure properties of ZnO. *Journal of Applied Physics*, **1998**, 83, 8065-8067	2.5	90
663	Electronic structure of two-dimensional transition metal dichalcogenide bilayers from ab initio theory. *Physical Review B*, **2014**, 89,	3.3	88
662	Photoemission and the electronic structure of PuCoGa5. *Physical Review Letters*, **2003**, 91, 176401	7.4	86
661	Fermi condensation near van Hove singularities within the Hubbard model on the triangular lattice. *Physical Review Letters*, **2014**, 112, 070403	7.4	84
660	The self-consistent ab initio lattice dynamical method. *Computational Materials Science*, **2009**, 44, 888-894	3.2	84
659	Theory of phase stabilities and bonding mechanisms in stoichiometric and substoichiometric molybdenum carbide. *Journal of Applied Physics*, **1999**, 86, 3758-3767	2.5	84
658	Orbital Magnetism and Magnetic Anisotropy Probed with Ferromagnetic Resonance. *Physical Review Letters*, **1999**, 82, 2390-2393	7.4	82
657	Charge self-consistent dynamical mean-field theory based on the full-potential linear muffin-tin orbital method: Methodology and applications. *Computational Materials Science*, **2012**, 55, 295-302	3.2	81
656	Predicting breast cancer recurrence. *Cancer*, **1982**, 50, 2884-93	6.4	80
655	Conductivity engineering of graphene by defect formation. *Journal Physics D: Applied Physics*, **2010**, 43, 045404	3	79
654	Spin-orbit coupling in the actinide elements: A critical evaluation of theoretical equilibrium volumes. *Physical Review B*, **2000**, 63,	3.3	77
653	Design of Nanocomposite Low-Friction Coatings. *Advanced Functional Materials*, **2007**, 17, 1611-1616	15.6	76
652	Phase stabilities and homogeneity ranges in 4d-transition-metal carbides: A theoretical study. *Physical Review B*, **2001**, 63,	3.3	76

651	Theoretical and experimental study of the graphite 1s x-ray absorption edges. *Physical Review B*, **1996**, 54, 14396-14404	3.3	76
650	Magnetic coupling in 3d transition-metal monolayers and bilayers on bcc (100) iron. *Physical Review B*, **1995**, 52, 15070-15073	3.3	73
649	Sum rules for electron energy loss near edge spectra. *Physical Review B*, **2007**, 76,	3.3	72
648	Computerized nuclear morphometry as an objective method for characterizing human cancer cell populations. *Cancer Research*, **1978**, 38, 4688-97	10.1	72
647	Calculation of uniaxial magnetic anisotropy energy of tetragonal and trigonal Fe, Co, and Ni. *Physical Review B*, **2004**, 69,	3.3	71
646	Spin and orbital contributions to surface magnetism in 3d elements. *Physical Review B*, **1992**, 45, 2868-2875	3.3	71
645	A novel electronic configuration of the 5f states in δ-plutonium as revealed by the photo-electron spectra. *Journal of Electron Spectroscopy and Related Phenomena*, **2004**, 135, 163-166	1.7	70
644	Chemical bonding and magnetism in 3d-5f intermetallics. *Journal of Physics F: Metal Physics*, **1988**, 18, L33-L39		70
643	Efficient spin injection through exchange coupling at organic semiconductor/ferromagnet heterojunctions. *Advanced Materials*, **2010**, 22, 1626-30	24	69
642	Optical properties of monoclinic SnI2 from relativistic first-principles theory. *Physical Review B*, **1997**, 56, 6851-6861	3.3	68
641	Modeling the actinides with disordered local moments. *Physical Review B*, **2003**, 67,	3.3	68
640	Theoretical confirmation of the high pressure simple cubic phase in calcium. *Physical Review Letters*, **1995**, 75, 3473-3476	7.4	68
639	Atomistic Spin Dynamics **2017**,		67
638	Complex edge effects in zigzag graphene nanoribbons due to hydrogen loading. *Physical Review B*, **2010**, 82,	3.3	65
637	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
636	Density functional study of elastic and vibrational properties of the Heusler-type alloys Fe2VAl and Fe2VGa. *Physical Review B*, **2009**, 80,	3.3	64
635	Theoretical Aspects of the Charge Density Wave in Uranium. *Physical Review Letters*, **1998**, 81, 2978-2981	7.4	64
634	Histopathological systems of breast cancer classification: reproducibility and clinical significance. *Journal of Clinical Pathology*, **1983**, 36, 392-8	3.9	64

633	Graphene as a reversible spin manipulator of molecular magnets. *Physical Review Letters*, **2011**, 107, 257202	7.4	63
632	Phase stability diagrams of transition metal carbides, a theoretical study. *Chemical Physics Letters*, **2001**, 333, 444-450	2.5	63
631	Magnetically induced crystal structure and phase stability in Fe1-cCoc. *Physical Review B*, **1996**, 54, 3380-3384	3.3	63
630	Origin of magnetic anisotropy of Gd metal. *Physical Review Letters*, **2003**, 91, 157201	7.4	62
629	Evolving properties of two-dimensional materials: from graphene to graphite. *Journal of Physics Condensed Matter*, **2009**, 21, 335502	1.8	61
628	Magnetic and electronic structure of (Ga1MnxAs. *Physical Review B*, **2003**, 67,	3.3	61
627	Electronic structure of Ti3SiC2. *Applied Physics Letters*, **2000**, 76, 2226-2228	3.4	61
626	Electronic, quasiharmonic, and anharmonic entropies of transition metals. *Physical Review B*, **1992**, 46, 5221-5228	3.3	61
625	Interatomic exchange interactions for finite-temperature magnetism and nonequilibrium spin dynamics. *Physical Review Letters*, **2013**, 111, 127204	7.4	60
624	Topological excitations in a kagome magnet. *Nature Communications*, **2014**, 5, 4815	17.4	57
623	Phonon spectrum, thermodynamic properties, and pressure-temperature phase diagram of uranium dioxide. *Physical Review B*, **2013**, 88,	3.3	57
622	Bonding mechanism in the nitrides Ti2AlN and TiN: An experimental and theoretical investigation. *Physical Review B*, **2007**, 76,	3.3	56
621	Balanced crystal orbital overlap population tool for analysing chemical bonds in solids. *Journal of Physics Condensed Matter*, **2003**, 15, 7751-7761	1.8	56
620	Magnetic properties and disorder effects in diluted magnetic semiconductors. *Physical Review B*, **2005**, 72,	3.3	55
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618	Electronic structure of graphite: Effect of hydrostatic pressure. *Physical Review B*, **1995**, 51, 4813-4819	3.3	55
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616	Theory of spin-polarized scanning tunneling microscopy applied to local spins. *Physical Review B*, **2010**, 81,	3.3	54

615	On the semiconducting state and structural properties of YH3 from first principles theory. *Applied Physics Letters*, **1997**, 71, 3498-3500	3.4	54
614	Electronic structure and chemical bonding in Ti2AlC investigated by soft x-ray emission spectroscopy. *Physical Review B*, **2006**, 74,	3.3	54
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612	Improved gas sensing activity in structurally defected bilayer graphene. *Nanotechnology*, **2012**, 23, 505501	3.4	53
611	Cohesive properties of the lanthanides: Effect of generalized gradient corrections and crystal structure. *Physical Review B*, **1998**, 58, 4345-4351	3.3	53
610	Electronic entanglement in late transition metal oxides. *Physical Review Letters*, **2012**, 109, 186401	7.4	52
609	Dynamical stability of body center cubic iron at the Earth's core conditions. *Proceedings of the National Academy of Sciences of the United States of America*, **2010**, 107, 9962-4	11.5	52
608	Quantitative magnetic information from reciprocal space maps in transmission electron microscopy. *Physical Review Letters*, **2009**, 102, 037201	7.4	52
607	Electronic structure investigation of Ti3AlC2, Ti3SiC2, and Ti3GeC2 by soft x-ray emission spectroscopy. *Physical Review B*, **2005**, 72,	3.3	52
606	High-temperature phonon stabilization of □uranium from relativistic first-principles theory. *Physical Review B*, **2012**, 85,	3.3	51
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604	Method for Calculating Valence Stability in Lanthanide Systems. *Physical Review Letters*, **1997**, 79, 4637-4640	7.4	51
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602	Mapping the magnetic transition temperatures for medium- and high-entropy alloys. *Intermetallics*, **2018**, 95, 80-84	3.5	50
601	Ab initio theory of dynamical core-hole screening in graphite from x-ray absorption spectra. *Physical Review Letters*, **2005**, 94, 167401	7.4	50
600	Magnetic properties of (Fe1□Cox)2B alloys and the effect of doping by 5d elements. *Physical Review B*, **2015**, 92,	3.3	48
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597	Electronic Configuration of Yb Compounds. *Physical Review Letters*, **1999**, 83, 3900-3903	7.4	48
596	Isomer shifts and hyperfine fields in iron compounds. *Journal of Physics Condensed Matter*, **1989**, 1, 1589-1599	1.8	48
595	First-principles calculations of the ultralow thermal conductivity in two-dimensional group-IV selenides. *Physical Review B*, **2018**, 98,	3.3	48
594	Effects of spin-dependent quasiparticle renormalization in Fe, Co, and Ni photoemission spectra:An experimental and theoretical study. *Physical Review B*, **2012**, 85,	3.3	47
593	Valence-band electronic structure of iron phthalocyanine: an experimental and theoretical photoelectron spectroscopy study. *Journal of Chemical Physics*, **2011**, 134, 074312	3.9	47
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591	Electronic structure and bulk properties of MB6 and MB12 borides. *Low Temperature Physics*, **2008**, 34, 921-929	0.7	47
590	Crystal-field levels and magnetic susceptibility in PuO2. *Physical Review B*, **2002**, 65,	3.3	47
589	Electronic structure, magnetic, and cohesive properties of LixMn2O4:Theory. *Physical Review B*, **2002**, 65,	3.3	47
588	Chemical vapour deposition of molybdenum carbides: aspects of phase stability. *Thin Solid Films*, **2000**, 370, 203-212	2.2	47
587	Bulk and surface magnetism and interplanar spacings in Gd from first-principles calculations. *Physical Review B*, **1995**, 52, 4420-4426	3.3	47
586	Stabilization of the tetragonal distortion of FexCo1⊠ alloys by C impurities: A potential new permanent magnet. *Physical Review B*, **2014**, 89,	3.3	46
585	Conditions for noncollinear instabilities of ferromagnetic materials. *Physical Review Letters*, **2004**, 93, 107205	7.4	46
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583	Standard model of the rare earths analyzed from the Hubbard I approximation. *Physical Review B*, **2016**, 94,	3.3	45
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577	Electronic structure and chemical and magnetic interactions in ZnO doped with Co and Al: Experiments and ab initio density-functional calculations. *Physical Review B*, **2008**, 78,	3.3	44
576	Delocalization and new phase in americium: Density-functional electronic structure calculations. *Physical Review B*, **2000**, 61, 8119-8124	3.3	44
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569	Many-body approach to spin-dependent transport in quantum dot systems. *Physical Review Letters*, **2002**, 88, 226601	7.4	43
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566	General trend of the mechanical properties of the ternary carbides M3SiC2 (M=transition metal). *Physical Review B*, **2006**, 74,	3.3	42
565	On the sharpness of the interfaces in metallic multilayers. *Proceedings of the National Academy of Sciences of the United States of America*, **2004**, 101, 4742-5	11.5	42
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561	Manipulation of spin state of iron porphyrin by chemisorption on magnetic substrates. *Physical Review B*, **2013**, 88,	3.3	40
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559	Electronic and optical properties of red HgI2. *Physical Review B*, **1996**, 54, 10419-10424	3.3	40
558	Magnetic interactions of Mn clusters supported on Cu. *Physical Review B*, **2006**, 73,	3.3	39
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
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551	Small gold clusters on graphene, their mobility and clustering: a DFT study. *Journal of Physics Condensed Matter*, **2011**, 23, 205301	1.8	37
550	Theory of He trapping, diffusion, and clustering in UO2. *Journal of Nuclear Materials*, **2009**, 385, 510-516	3.3	37
549	Electronic-structure calculations of praseodymium metal by means of modified density-functional theory. *Physical Review B*, **1997**, 56, 7143-7148	3.3	37
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