Per Sderlind

List of Publications by Citations

164 papers	5,342 citations	41 h-index	66 g-index
174 ext. papers	5,692 ext. citations	4.2 avg, IF	5.66 L-index

#	Paper	IF	Citations
164	First-principles theory of iron up to earth-core pressures: Structural, vibrational, and elastic properties. *Physical Review B*, **1996**, 53, 14063-14072	3.3	221
163	Theory of elastic constants of cubic transition metals and alloys. *Physical Review B*, **1993**, 48, 5844-5851	3.3	214
162	A unified picture of the crystal structures of metals. *Nature*, **1995**, 374, 524-525	50.4	172
161	Density-functional calculations of alpha, beta, gamma, delta, delta', and epsilon plutonium. *Physical Review Letters*, **2004**, 92, 185702	7.4	157
160	Theory of the crystal structures of cerium and the light actinides. *Advances in Physics*, **1998**, 47, 959-998	18.4	148
159	Ambient pressure phase diagram of plutonium: A unified theory for □Pu and □Pu. *Europhysics Letters*, **2001**, 55, 525-531	1.6	130
158	Electronic properties of f-electron metals using the generalized gradient approximation. *Physical Review B*, **1994**, 50, 7291-7294	3.3	125
157	Spin and orbital magnetism in Fe-Co and Co-Ni alloys. *Physical Review B*, **1992**, 45, 12911-12916	3.3	125
156	Quantum-based atomistic simulation of materials properties in transition metals. *Journal of Physics Condensed Matter*, **2002**, 14, 2825-2857	1.8	123
155	Density-functional investigation of magnetism in □Pu. *Physical Review B*, **2002**, 66,	3.3	118
154	New beta(fcc)-cobalt to 210 GPa. *Physical Review Letters*, **2000**, 84, 4132-5	7.4	112
153	Theoretical aspects of the FecNi1-c Invar alloy. *Physical Review B*, **1995**, 51, 1058-1063	3.3	112
152	First-principles elastic and structural properties of uranium metal. *Physical Review B*, **2002**, 66,	3.3	108
151	Crystal structure and elastic-constant anomalies in the magnetic 3d transition metals. *Physical Review B*, **1994**, 50, 5918-5927	3.3	103
150	High-pressure melting curves of argon, krypton, and xenon: deviation from corresponding states theory. *Physical Review Letters*, **2001**, 86, 5731-4	7.4	102
149	Accurate atomistic simulation of (a/2) <111> screw dislocations and other defects in bcc tantalum. *Philosophical Magazine A: Physics of Condensed Matter, Structure, Defects and Mechanical Properties*, **2001**, 81, 1355-1385		100
148	Trends of the elastic constants of cubic transition metals. *Physical Review Letters*, **1992**, 68, 2802-2805	7.4	93

147	Relativistic effects on the thermal expansion of the actinide elements. *Physical Review B*, **1990**, 42, 4544-4552	3.3	91
146	Structural properties of plutonium from first-principles theory. *Physical Review B*, **1997**, 55, 1997-2004	3.3	90
145	Phase diagram of uranium at high pressures and temperatures. *Physical Review B*, **1998**, 57, 10359-10362	3.3	85
144	First-principles formation energies of monovacancies in bcc transition metals. *Physical Review B*, **2000**, 61, 2579-2586	3.3	85
143	First-principles theory of Ta up to 10 Mbar pressure: Structural and mechanical properties. *Physical Review B*, **1998**, 57, 10340-10350	3.3	85
142	Spin-orbit coupling in the actinide elements: A critical evaluation of theoretical equilibrium volumes. *Physical Review B*, **2000**, 63,	3.3	77
141	Magnetically induced crystal structure and phase stability in Fe1-cCoc. *Physical Review B*, **1996**, 54, 3380-3384	3.3	63
140	Shear-induced anisotropic plastic flow from body-centred-cubic tantalum before melting. *Nature Materials*, **2009**, 8, 223-8	27	62
139	Fermi surface nesting and pre-martensitic softening in V and Nb at high pressures. *Journal of Physics Condensed Matter*, **2006**, 18, 5079-5085	1.8	62
138	Computational modeling of actinide materials and complexes. *MRS Bulletin*, **2010**, 35, 883-888	3.2	58
137	Emergence of strong exchange interaction in the actinide series: the driving force for magnetic stabilization of curium. *Physical Review Letters*, **2007**, 98, 236402	7.4	56
136	High-temperature phonon stabilization of □uranium from relativistic first-principles theory. *Physical Review B*, **2012**, 85,	3.3	51
135	Density-functional study of U□Mo and U□r alloys. *Journal of Nuclear Materials*, **2011**, 414, 132-137	3.3	50
134	Quantifying the importance of orbital over spin correlations in □u within density-functional theory. *Physical Review B*, **2008**, 77,	3.3	48
133	Bulk and surface magnetism and interplanar spacings in Gd from first-principles calculations. *Physical Review B*, **1995**, 52, 4420-4426	3.3	47
132	Density-functional study of the U□r system. *Journal of Alloys and Compounds*, **2009**, 478, 103-110	5.7	46
131	The phase diagram of cobalt at high pressure and temperature: the stability of -cobalt and new -cobalt. *Journal of Physics Condensed Matter*, **1998**, 10, L311-L318	1.8	46
130	Crystal stability and equation of state for Am: Theory. *Physical Review B*, **2005**, 72,	3.3	46

129	First-principles thermoelasticity of transition metals at high pressure: Tantalum prototype in the quasiharmonic limit. *Physical Review B*, **2006**, 74,	3.3	45
128	Delocalization and new phase in americium: Density-functional electronic structure calculations. *Physical Review B*, **2000**, 61, 8119-8124	3.3	44
127	Temperature-driven phase transitions from first principles including all relevant excitations: The fcc-to-bcc transition in Ca. *Physical Review B*, **2011**, 84,	3.3	43
126	Elastic properties of Pu metal and Pu-Ga alloys. *Physical Review B*, **2010**, 81,	3.3	42
125	Robust quantum-based interatomic potentials for multiscale modeling in transition metals. *Journal of Materials Research*, **2006**, 21, 563-573	2.5	42
124	Theoretical confirmation of a high-pressure rhombohedral phase in vanadium metal. *Physical Review B*, **2007**, 75,	3.3	42
123	Phonon and magnetic structure in δ-plutonium from density-functional theory. *Scientific Reports*, **2015**, 5, 15958	4.9	39
122	Ab initio calculations of elastic constants of the bcc V–Nb system at high pressures. *Journal of Physics and Chemistry of Solids*, **2006**, 67, 2056-2064	3.9	39
121	Xenon melting curve to 80 GPa and 5p-d hybridization. *Physical Review Letters*, **2005**, 95, 257801	7.4	37
120	dhcp as a possible new ?? phase of iron at high pressures and temperatures. *Physics Letters, Section A: General, Atomic and Solid State Physics*, **1996**, 214, 65-70	2.3	37
119	Elastic constants of cubic f-electron elements: Theory. *Physical Review B*, **1993**, 48, 9306-9312	3.3	37
118	Symmetry and stability of plutonium: the influence of electronic structure. *Physical Review Letters*, **2006**, 96, 206402	7.4	36
117	Geometry and electronic structure of β-Pu: A theoretical study. *Physical Review B*, **2003**, 68,	3.3	36
116	Theoretical predictions of structural phase transitions in Cr, Mo, and W. *Physical Review B*, **1994**, 49, 9365-9371	3.3	36
115	On the electronic configuration in Pu: spectroscopy and theory. *Journal of Physics Condensed Matter*, **2008**, 20, 125204	1.8	35
114	Changes in the electronic structure of cerium due to variations in close packing. *Physical Review B*, **2004**, 69,	3.3	32
113	fcc-->bct phase transition in Th at extreme compressions: Theory. *Physical Review B*, **1992**, 45, 12588-12591	3.3	32
112	First-principles elastic constants and phonons of β-Pu. *Physical Review B*, **2004**, 70,	3.3	30

111	Electron correlation and relativity of the 5f electrons in the U□r alloy system. *Journal of Nuclear Materials*, **2014**, 444, 356-358	3.3	29
110	First-principles phase stability, bonding, and electronic structure of actinide metals. *Journal of Electron Spectroscopy and Related Phenomena*, **2014**, 194, 2-7	1.7	29
109	Stability in bcc transition metals: Madelung and band-energy effects due to alloying. *Physical Review Letters*, **2009**, 103, 235501	7.4	29
108	Delocalization and phase transitions in Pr: Theory. *Physical Review B*, **2002**, 65,	3.3	29
107	Prediction of the new efficient permanent magnet SmCoNiFe3. *Physical Review B*, **2017**, 96,	3.3	28
106	Comment on □orrelation and relativistic effects in U metal and U-Zr alloy: Validation of ab initio approaches□*Physical Review B*, **2014**, 90,	3.3	28
105	Theoretical investigation of the high-pressure crystal structures of Ce and Th. *Physical Review B*, **1995**, 52, 13169-13176	3.3	28
104	Theoretical zero-temperature phase diagram for neptunium metal. *Physical Review B*, **1995**, 52, 1631-1639	3.3	28
103	Density-functional theory for plutonium. *Advances in Physics*, **2019**, 68, 1-47	18.4	27
102	First-principles elastic properties of □Pu. *Physical Review B*, **2009**, 79,	3.3	27
101	Atomistic simulation of pressure-dependent screw dislocation properties in bcc tantalum. *Materials Science & Engineering A: Structural Materials: Properties, Microstructure and Processing*, **2001**, 309-310, 102-107	5.3	27
100	The U□i system: Strengths and weaknesses of the CALPHAD method. *Journal of Nuclear Materials*, **2011**, 419, 177-185	3.3	26
99	Ground-state properties of rare-earth metals: an evaluation of density-functional theory. *Journal of Physics Condensed Matter*, **2014**, 26, 416001	1.8	25
98	Structural stability in uranium. *Journal of Physics Condensed Matter*, **1997**, 9, L549-L555	1.8	25
97	Influence of pseudocore valence-band hybridization on the crystal-structure phase stabilities of transition metals under extreme compressions. *Physical Review B*, **1994**, 50, 14690-14693	3.3	24
96	Pressure-induced phase transitions in Pa metal from first-principles theory. *Physical Review B*, **1997**, 56, 10719-10721	3.3	23
95	Monte Carlo simulations of the stability of □Pu. *Journal of Physics Condensed Matter*, **2003**, 15, L371-L376	1.8	23
94	Origin of the multiple configurations that drive the response of □plutonium's elastic moduli to temperature. *Proceedings of the National Academy of Sciences of the United States of America*, **2016**, 113, 11158-11161	11.5	23

93	Assessing a solids-biased density-gradient functional for actinide metals. *Physical Review B*, **2010**, 82,	3.3	22
92	Electron-energy-loss spectroscopy and X-ray absorption spectroscopy as complementary probes for complex f-electron metals: cerium and plutonium. *Philosophical Magazine*, **2004**, 84, 1039-1056	1.6	22
91	Density-functional calculations for cerium metal. *Physical Review B*, **1995**, 51, 4618-4621	3.3	22
90	Shear softening in tantalum at megabar pressures. *Physical Review B*, **2010**, 82,	3.3	21
89	Simple model for complex structures. *Physical Review B*, **1998**, 57, 1320-1323	3.3	21
88	Atomistic Simulations for Multiscale Modeling in bcc Metals. *Journal of Engineering Materials and Technology, Transactions of the ASME*, **1999**, 121, 120-125	1.8	21
87	Thermodynamics of SmCo5 compound doped with Fe and Ni: An ab initio study. *Journal of Alloys and Compounds*, **2018**, 765, 659-663	5.7	21
86	Stability of δ-Pu alloys from first-principles theory. *Journal of Alloys and Compounds*, **2003**, 354, 99-103	5.7	20
85	Density changes in Ga-stabilized δ-Pu, and what they mean. *Journal of Alloys and Compounds*, **2007**, 444-445, 72-79	5.7	18
84	Density-functional study of Zr-based actinide alloys: 2. U-Pu-Zr system. *Journal of Nuclear Materials* , **2009**, 393, 141-145	3.3	17
83	Pressure-induced changes in the electronic structure of americium metal. *Physical Review B*, **2011**, 84,	3.3	17
82	Kohn Anomaly and Phase Stability in Group VB Transition Metals. *Computation*, **2018**, 6, 29	2.2	16
81	Thermodynamic re-assessment of the Pu-U system and its application to the ternary Pu-U-Ga system. *Journal of Nuclear Materials*, **2014**, 454, 81-95	3.3	16
80	An alternative model for electron correlation in Pu. *Journal of Physics Condensed Matter*, **2008**, 20, 422202	2.8	16
79	First principles studies of crystal structures of f elements. *Physica B: Condensed Matter*, **1993**, 190, 5-11	2.8	16
78	Density-functional study of Zr-based actinide alloys. *Journal of Nuclear Materials*, **2009**, 385, 68-71	3.3	15
77	Calculated thermal expansion of d and f transition metals. *Thermochimica Acta*, **1993**, 218, 145-153	2.9	15
76	Zero-Kelvin Compression Isotherms of the Elements 1 ≤ Z ≤ 92 to 100 GPa. *Journal of Physical and Chemical Reference Data*, **2016**, 45, 043101	4.3	14

75	Development of a CALPHAD Thermodynamic Database for Pu-U-Fe-Ga Alloys. *Applied Sciences (Switzerland)*, **2019**, 9, 5040	2.6	14
74	The Pu–U–Am system: An ab initio informed CALPHAD thermodynamic study. *Journal of Nuclear Materials*, **2015**, 458, 425-441	3.3	13
73	When magnetism can stabilize the crystal structure of metals. *Scripta Materialia*, **2008**, 59, 1259-1262	5.6	13
72	Assessing Relativistic Effects and Electron Correlation in the Actinide Metals Th to Pu. *Applied Sciences (Switzerland)*, **2019**, 9, 5020	2.6	13
71	Ab initio phase stability at high temperatures and pressures in the V-Cr system. *Physical Review B*, **2014**, 89,	3.3	12
70	Thermodynamic modeling of chromium: strong and weak magnetic coupling. *Journal of Physics Condensed Matter*, **2013**, 25, 425401	1.8	12
69	Cancellation of spin and orbital magnetic moments in δ-Pu: Theory. *Journal of Alloys and Compounds*, **2007**, 444-445, 93-97	5.7	12
68	Local-moment collapse in compressed samarium metal. *Physical Review B*, **1993**, 48, 9212-9215	3.3	12
67	Crystallographic phase transitions in actinide metals as a function of pressure. *Journal of Alloys and Compounds*, **1994**, 213-214, 268-277	5.7	12
66	First-principles phase stability in the Ti-V alloy system. *Journal of Alloys and Compounds*, **2013**, 581, 856-859	5.7	11
65	Density-functional study of bcc U–Mo, Np–Mo, Pu–Mo, and Am–Mo alloys. *Journal of Nuclear Materials*, **2013**, 434, 31-37	3.3	11
64	Volume changes in δ-plutonium from helium and other decay products. *Journal of Nuclear Materials* , **2006**, 355, 21-29	3.3	11
63	Simple model for localization in δ-Pu. *Modelling and Simulation in Materials Science and Engineering*, **2003**, 11, 851-858	2	11
62	First-principles calculations of stability of δ-Pu–Am alloys. *Journal of Alloys and Compounds*, **2004**, 376, 62-67	5.7	11
61	Anharmonicity-induced first-order isostructural phase transition of zirconium under pressure. *Physical Review B*, **2018**, 98,	3.3	11
60	Assessing Density-Functional Theory for Equation-Of-State. *Computation*, **2018**, 6, 13	2.2	11
59	Elastic moduli of δ-Pu239 reveal aging in real time. *Journal of Applied Physics*, **2017**, 121, 125107	2.5	10
58	Theoretical confirmation of Ga-stabilized anti-ferromagnetism in plutonium metal. *Journal of Nuclear Materials*, **2014**, 448, 310-314	3.3	10

57	Thermodynamic assessment of the AmPu system with input from ab initio. *Journal of Nuclear Materials*, **2011**, 418, 165-173	3.3	10
56	First-principles phase diagram of the Ce-Th system. *Physical Review B*, **2004**, 70,	3.3	10
55	Comment on Theoretical prediction of phase transition in gold *Physical Review B*, **2002**, 66,	3.3	10
54	Ground-State and Thermodynamical Properties of Uranium Mononitride from Anharmonic First-Principles Theory. *Applied Sciences (Switzerland)*, **2019**, 9, 3914	2.6	9
53	Magnetism and structural distortions in uranium sulfide under pressure. *Physical Review B*, **2013**, 87,	3.3	9
52	Density-functional study of bcc PuU, PuNp, PuAm, and PuCm alloys. *Journal of Nuclear Materials*, **2011**, 408, 61-66	3.3	9
51	Density-functional electronic structure of PuCoGa5. *Physical Review B*, **2004**, 70,	3.3	9
50	A theoretical study of the crystallographic structures in neptunium. *Journal of Physics Condensed Matter*, **1994**, 6, 6573-6580	1.8	9
49	Lattice dynamics and elasticity for plutonium. *Scientific Reports*, **2017**, 7, 1116	4.9	8
48	Thermodynamic study of the NpZr system. *Journal of Nuclear Materials*, **2011**, 409, 1-8	3.3	8
47	Accurate atomistic simulation of (a/2) <111> screw dislocations and other defects in bcc tantalum		8
46	On the valence fluctuation in the early actinide metals. *Journal of Electron Spectroscopy and Related Phenomena*, **2016**, 207, 14-18	1.7	7
45	From Electronic Structure to Thermodynamics of Actinide-Based Alloys. *Jom*, **2014**, 66, 375-388	2.1	7
44	Rubidium at high pressure and temperature. *Journal of Physics Condensed Matter*, **2000**, 12, 921-931	1.8	7
43	Theoretical study of the pressure-concentration diagram for the Ce-Th alloy system. *Physical Review B*, **1999**, 60, 9372-9376	3.3	7
42	Alloying-driven phase stability in group-VB transition metals under compression. *Physical Review B*, **2010**, 82,	3.3	6
41	Incorporating anisotropic electronic structure in crystallographic determination of complex metals: iron and plutonium. *Philosophical Magazine*, **2007**, 87, 2571-2588	1.6	6
40	Fermi surface of noble metals: Full-potential generalized-gradient-approximation calculations. *Physical Review B*, **1994**, 50, 11183-11186	3.3	6

39	Electronic structure of platinum at ultrahigh pressure. *High Pressure Research*, **1994**, 12, 161-170	1.6	6
38	Spin and orbital magnetism in Fe?Co and Co?Ni alloys. *Journal of Magnetism and Magnetic Materials*, **1992**, 104-107, 2037-2039	2.8	6
37	Phonon dispersion of Mo-stabilized -U measured using inelastic x-ray scattering. *Physical Review B*, **2019**, 100,	3.3	5
36	First-principles phase stability at high temperatures and pressure in Nb90Zr10 alloy. *Journal of Alloys and Compounds*, **2017**, 690, 647-651	5.7	5
35	Comment on "new pseudophase structure for alpha-Pu". *Physical Review Letters*, **2004**, 93, 199601; author reply 199602	7.4	5
34	Reply to Janoschek et al.: The excited □phase of plutonium. *Proceedings of the National Academy of Sciences of the United States of America*, **2017**, 114, E269	11.5	4
33	Phase Stability in U-6Nb Alloy Doped with Ti from the First Principles Theory. *Applied Sciences (Switzerland)*, **2020**, 10, 3417	2.6	4
32	Formation of high purity uranium via laser induced thermal decomposition of uranium nitride. *Materials and Design*, **2020**, 192, 108706	8.1	4
31	Fermi surface of alkali metals using the full-potential linear muffin-tin orbital method and the generalized gradient approximation. *Physical Review B*, **1994**, 50, 18003-18006	3.3	4
30	Electronically driven volume collapses of bantam-heavy actinide elements at high pressure. *Physica B: Condensed Matter*, **1993**, 190, 12-20	2.8	4
29	Phonon density of states for □plutonium from density-functional theory. *Scientific Reports*, **2019**, 9, 18682	4.9	4
28	Atomic-volume variations of □Pu alloyed with Al, Ga, and Am from first-principles theory. *Journal of Computer-Aided Materials Design*, **2007**, 14, 349-355		3
27	Calculated thermal expansion of the actinide elements. *International Journal of Thermophysics*, **1991**, 12, 611-615	2.1	3
26	Thermodynamics of Plutonium Monocarbide from Anharmonic and Relativistic Theory. *Applied Sciences (Switzerland)*, **2020**, 10, 6524	2.6	3
25	The ultrahigh pressure stability of silver: An experimental and theoretical study. *Journal of Applied Physics*, **2021**, 129, 125901	2.5	3
24	Thermodynamics of Uranium Tri-Iodide from Density-Functional Theory. *Applied Sciences (Switzerland)*, **2020**, 10, 3914	2.6	2
23	Density-functional calculations of □Pu□a(Al) alloys. *Journal of Alloys and Compounds*, **2007**, 444-445, 296-299	5.7	2
22	Relativistic effects on the equation of state of the light actinides. *Materials Research Society Symposia Proceedings*, **2005**, 893, 1		2

21	Thermodynamics and Magnetism of YCo5 Compound Doped with Fe and Ni: An Ab Initio Study. *Applied Sciences (Switzerland)*, **2020**, 10, 6037	2.6	2
20	Mechanical and Thermal Properties for Uranium and U–Nb Alloy from First-Principles Theory. *Applied Sciences (Switzerland)*, **2021**, 11, 5643	2.6	2
19	Pressure-dependent intermediate valence behavior in YbNiGa4 and YbNiIn4. *Physical Review B*, **2018**, 98,	3.3	2
18	Thermodynamics and Magnetism of SmFe12 Compound Doped with Co and Ni: An Ab Initio Study. *Applied Sciences (Switzerland)*, **2022**, 12, 4860	2.6	2
17	High Pressure and Temperature Elasticity and EOS for Actinide Metals from First-Principles Simulations. *Materials Research Society Symposia Proceedings*, **2014**, 1683, 44		1
16	Ab Initio Study of Advanced Metallic Nuclear Fuels for Fast Breeder Reactors□CORRIGENDUM. *Materials Research Society Symposia Proceedings*, **2012**, 1444, 1-1		1
15	Quantifying the Importance of Orbital Over Spin Correlations in □Pu Within Density-Functional Theory. *Materials Research Society Symposia Proceedings*, **2008**, 1104, 1		1
14	Phase stability in heavy f-electron metals from first-principles theory. *Materials Research Society Symposia Proceedings*, **2005**, 893, 1		1
13	ELASTIC CONSTANTS OF d TRANSITION ELEMENTS AND d TRANSITION ALLOYS. *International Journal of Modern Physics B*, **1993**, 07, 203-206	1.1	1
12	Thermodynamics Modeling for Actinide Monocarbides and Mononitrides from First Principles. *Applied Sciences (Switzerland)*, **2022**, 12, 728	2.6	1
11	High pressure stability of □Zr: no evidence for isostructural phase transitions. *High Pressure Research*, **2021**, 41, 247-266	1.6	1
10	Theoretical confirmation of Ga-stabilized anti-ferromagnetism in plutonium metal. *Materials Research Society Symposia Proceedings*, **2014**, 1683, 21		
9	Ab Initio Study of Advanced Metallic Nuclear Fuels for Fast Breeder Reactors. *Materials Research Society Symposia Proceedings*, **2012**, 1444, 67		
8	Alloying-Driven Phase Stability in Group-VB Transition Metals under Compression. *Materials Research Society Symposia Proceedings*, **2011**, 1369, 1		
7	First-principles electronic and elastic properties of plutonium metal. *IOP Conference Series: Materials Science and Engineering*, **2010**, 9, 012083	0.4	
6	On the electronic configuration in Pu. *Materials Research Society Symposia Proceedings*, **2006**, 986, 1		
5	Electronic structure calculations of □Pu based alloys. *Materials Research Society Symposia Proceedings*, **2003**, 802, 209		
4	Symmetry reduction of □plutonium: an electronic-structure effect. *Materials Research Society Symposia Proceedings*, **2005**, 893, 1		

List of Publications

3	Magnetic effects on structural, elastic and surface properties of the 3d ferromagnets. *Journal of Magnetism and Magnetic Materials*, **1995**, 140-144, 29-33	2.8
2	Crystal Structure and Phase Stability in Fe1-xCox from AB Initio Theory **1997**, 13-17	
1	Alloying-Driven Phase Stability in Group-VB Transition Metals under Compression. *Solid State Phenomena*, **2016**, 258, 125-130	0.4