Ole Martin Lvvik

List of Publications by Year in Descending Order

129 papers	3,386 citations	32 h-index	54 g-index
132 ext. papers	3,750 ext. citations	3.9 avg, IF	5.44 L-index

#	Paper	IF	Citations
129	Attaining Low Lattice Thermal Conductivity in Half-Heusler Sublattice Solid Solutions: Which Substitution Site Is Most Effective?. *Electronic Materials*, **2022**, 3, 1-14	0.8	
128	High entropy alloy CrFeNiCoCu sputter deposited films: Structure, electrical properties, and oxidation. *Journal of Vacuum Science and Technology A: Vacuum, Surfaces and Films*, **2022**, 40, 023402	2.9	
127	Lattice thermal conductivity of half-Heuslers with density functional theory and machine learning: Enhancing predictivity by active sampling with principal component analysis. *Computational Materials Science*, **2022**, 202, 110938	3.2	3
126	New structure and insight on the phase transition within the Cu-Pd-Sn system with 25 at. % Sn.. *Materialia*, **2022**, 101461	3.2	
125	Fabrication of a Silicide Thermoelectric Module Employing Fractional Factorial Design Principles. *Journal of Electronic Materials*, **2021**, 50, 4041-4049	1.9	2
124	Jahn-Teller active fluoroperovskites ACrF3 (A=Na+,K+): Magnetic and thermo-optical properties. *Physical Review Materials*, **2021**, 5,	3.2	1
123	Discarded gems: Thermoelectric performance of materials with band gap emerging at the hybrid-functional level. *Applied Physics Letters*, **2021**, 119, 081902	3.4	0
122	Vacancy diffusion in palladium hydrides. *Physical Chemistry Chemical Physics*, **2021**, 23, 13680-13686	3.6	0
121	Hydrogen induced vacancy clustering and void formation mechanisms at grain boundaries in palladium. *Acta Materialia*, **2020**, 195, 708-719	8.4	10
120	Structural and magnetic characterization of the elusive Jahn-Teller active NaCrF3. *Physical Review Materials*, **2020**, 4,	3.2	2
119	Screening of thermoelectric silicides with atomistic transport calculations. *Journal of Applied Physics*, **2020**, 128, 125105	2.5	0
118	Calculation of the anisotropic coefficients of thermal expansion: A first-principles approach. *Computational Materials Science*, **2019**, 167, 257-263	3.2	8
117	Application of machine learning-based selective sampling to determine BaZrO3 grain boundary structures. *Computational Materials Science*, **2019**, 164, 57-65	3.2	4
116	Determining the Optimal Phase-Change Material via High-Throughput Calculations. *MRS Advances*, **2019**, 4, 2679-2687	0.7	2
115	A Review of Eutectic Au-Ge Solder Joints. *Metallurgical and Materials Transactions A: Physical Metallurgy and Materials Science*, **2019**, 50, 4632-4641	2.3	2
114	Investigation of the electrostatic potential of a grain boundary in Y-substituted BaZrO using inline electron holography. *Physical Chemistry Chemical Physics*, **2019**, 21, 17662-17672	3.6	3
113	Thermoelectric transport trends in group 4 half-Heusler alloys. *Journal of Applied Physics*, **2019**, 126, 145102	2.5	15

112	Effectiveness of Neural Networks for Research on Novel Thermoelectric Materials. A Proof of Concept. *Communications in Computer and Information Science*, **2019**, 69-77	0.3	
111	Decohesion Energy of (Sigma 5(012)) Grain Boundaries in Ni as Function of Hydrogen Content. *Metallurgical and Materials Transactions A: Physical Metallurgy and Materials Science*, **2019**, 50, 451-456	2.3	2
110	Segregation of Mg, Cu and their effects on the strength of Al Σ5 (210)[001] symmetrical tilt grain boundary. *Acta Materialia*, **2018**, 145, 235-246	8.4	59
109	Formation of nanoporous Si upon self-organized growth of Al and Si nanostructures. *Nanotechnology*, **2018**, 29, 315602	3.4	5
108	Leakage evolution and atomic-scale changes in Pd-based membranes induced by long-term hydrogen permeation. *Journal of Membrane Science*, **2018**, 563, 398-404	9.6	19
107	Boron-doping of cubic SiC for intermediate band solar cells: a scanning transmission electron microscopy study. *SciPost Physics*, **2018**, 5,	6.1	2
106	Valence charge distribution in homogenous silicon-aluminium thin-films. *Journal of Physics Condensed Matter*, **2018**, 30, 335502	1.8	1
105	Optical and Microstructural Investigation of Heavy B-Doping Effects in Sublimation-Grown 3C-SiC. *Materials Science Forum*, **2018**, 924, 221-224	0.4	1
104	Discovering Thermoelectric Materials Using Machine Learning: Insights and Challenges. *Lecture Notes in Computer Science*, **2018**, 392-401	0.9	4
103	Grain Boundary Segregation in Pd-Cu-Ag Alloys for High Permeability Hydrogen Separation Membranes. *Membranes*, **2018**, 8,	3.8	4
102	Predicting the thermoelectric figure-of-merit from first principles. *Materials Today: Proceedings*, **2018**, 5, 10227-10234	1.4	5
101	Lattice thermal conductivity of TixZryHf1−x−yNiSn half-Heusler alloys calculated from first principles: Key role of nature of phonon modes. *Physical Review B*, **2017**, 95,	3.3	59
100	Optimising multi-frame ADF-STEM for high-precision atomic-resolution strain mapping. *Ultramicroscopy*, **2017**, 179, 57-62	3.1	36
99	The role of grain boundary scattering in reducing the thermal conductivity of polycrystalline XNiSn (X = Hf, Zr, Ti) half-Heusler alloys. *Scientific Reports*, **2017**, 7, 13760	4.9	43
98	Characterization of B-Implanted 3C-SiC for Intermediate Band Solar Cells. *Materials Science Forum*, **2017**, 897, 299-302	0.4	1
97	Interface phenomena in magnetron sputtered CuO/ZnO heterostructures. *Journal of Physics Condensed Matter*, **2017**, 29, 435002	1.8	2
96	Twinnability of Al–Mg alloys: A first-principles interpretation. *Transactions of Nonferrous Metals Society of China*, **2017**, 27, 1313-1318	3.3	2
95	Combined effect of Mg and vacancy on the generalized planar fault energy of Al. *Journal of Alloys and Compounds*, **2017**, 690, 841-850	5.7	14

94	Thermoelectric module for high temperature application **2017**,		2
93	Mapping the Chemistry Within, and the Strain Around, Al-alloy Precipitates at Atomic Resolution by Multi-frame Scanning Transmission Electron Microscopy. *Microscopy and Microanalysis*, **2017**, 23, 384-385	0.5	
92	Atomic scale study of Cu2O/ZnO heterojunction interfaces by TEM, STEM and DFT **2016**, 676-677		
91	Comparing electrochemical performance of transition metal silicate cathodes and chevrel phase Mo6S8 in the analogous rechargeable Mg-ion battery system. *Journal of Power Sources*, **2016**, 321, 76-86	8.9	20
90	Boron-Implanted 3C-SiC for Intermediate Band Solar Cells. *Materials Science Forum*, **2016**, 858, 291-294	0.4	5
89	Nanocomposites of few-layer graphene oxide and alumina by density functional theory calculations. *Journal of the European Ceramic Society*, **2016**, 36, 719-724	6	10
88	Cubic silicon carbide as a potential photovoltaic material. *Solar Energy Materials and Solar Cells*, **2016**, 145, 104-108	6.4	32
87	Structural properties of Cu2O epitaxial films grown on c-axis single crystal ZnO by magnetron sputtering. *Applied Physics Letters*, **2016**, 108, 152110	3.4	9
86	Enhancement of thermoelectric properties by energy filtering: Theoretical potential and experimental reality in nanostructured ZnSb. *Journal of Applied Physics*, **2016**, 119, 125103	2.5	25
85	Direct-to-indirect bandgap transitions in <110> silicon nanowires. *Journal of Applied Physics*, **2016**, 119, 015702	2.5	15
84	Impurity effect of Mg on the generalized planar fault energy of Al. *Journal of Materials Science*, **2016**, 51, 6552-6568	4.3	31
83	Epitaxial Strain-Induced Growth of CuO at Cu2O/ZnO Interfaces. *Journal of Physical Chemistry C*, **2016**, 120, 23552-23558	3.8	11
82	Nanostructuring of Undoped ZnSb by Cryo-Milling. *Journal of Electronic Materials*, **2015**, 44, 2578-2584	1.9	14
81	Hydrogen embrittlement in nickel, visited by first principles modeling, cohesive zone simulation and nanomechanical testing. *International Journal of Hydrogen Energy*, **2015**, 40, 16892-16900	6.7	69
80	Multi-component solid solution and cluster hardening of Al□Mn□Si alloys. *Materials Science & Engineering A: Structural Materials: Properties, Microstructure and Processing*, **2015**, 625, 153-157	5.3	14
79	Density Functional Study of the □ Phase in Al-Mg-Si Alloys. *Metallurgical and Materials Transactions A: Physical Metallurgy and Materials Science*, **2014**, 45, 2916-2924	2.3	16
78	Initial stages of ITO/Si interface formation: In situ x-ray photoelectron spectroscopy measurements upon magnetron sputtering and atomistic modelling using density functional theory. *Journal of Applied Physics*, **2014**, 115, 083705	2.5	13
77	Removal of Phosphorus in Metallurgical Silicon by Rare Earth Elements. *Metallurgical and Materials Transactions E*, **2014**, 1, 257-262		1

76	Oxygen Nonstoichiometry in (Ca2CoO3)0.62(CoO2): A Combined Experimental and Computational Study. *Journal of Physical Chemistry C*, **2014**, 118, 18899-18907	3.8	22
75	Prediction of solute diffusivity in Al assisted by first-principles molecular dynamics. *Journal of Physics Condensed Matter*, **2014**, 26, 025403	1.8	5
74	Perovskite to postperovskite transition in NaFeF3. *Inorganic Chemistry*, **2014**, 53, 12205-14	5.1	14
73	Detailed atomistic insight into the β′ phase in Al–Mg–Si alloys. *Acta Materialia*, **2014**, 69, 126-134	8.4	115
72	First-principles calculations on sulfur interacting with ternary Pd–Ag-transition metal alloy membrane alloys. *Journal of Membrane Science*, **2014**, 453, 525-531	9.6	15
71	X-ray photoelectron spectroscopy investigation of magnetron sputtered Mg–Ti–H thin films. *International Journal of Hydrogen Energy*, **2013**, 38, 10704-10715	6.7	16
70	Effect of Temperature on the Die Shear Strength of a Au-Sn SLID Bond. *Metallurgical and Materials Transactions A: Physical Metallurgy and Materials Science*, **2013**, 44, 2914-2916	2.3	21
69	High Temperature Interconnect and Die Attach Technology: Au–Sn SLID Bonding. *IEEE Transactions on Components, Packaging and Manufacturing Technology*, **2013**, 3, 904-914	1.7	35
68	On the Complex Structural Picture of the Ionic Conductor Sr6Ta2O11. *Journal of Physical Chemistry C*, **2013**, 117, 9543-9549	3.8	6
67	Effect of Transition Metal Dopants on Initial Mass Transport in the Dehydrogenation of NaAlH4: Density Functional Theory Study. *Journal of Physical Chemistry C*, **2013**, 117, 3-14	3.8	18
66	β-Si3N4(0001)/Si(111) interface: Phosphorus defects, valence band offsets, and their role of passivating the interface states. *Physical Review B*, **2013**, 88,	3.3	11
65	Interfacial Charge Transfer and Chemical Bonding in a Ni–LaNbO4 Cermet for Proton-Conducting Solid-Oxide Fuel Cell Anodes. *Chemistry of Materials*, **2012**, 24, 4152-4159	9.6	14
64	Combined XPS and first principle study of metastable Mg–Ti thin films. *Surface and Interface Analysis*, **2012**, 44, 986-988	1.5	6
63	Au-Sn SLID Bonding—Properties and Possibilities. *Metallurgical and Materials Transactions B: Process Metallurgy and Materials Processing Science*, **2012**, 43, 397-405	2.5	64
62	Hydrogen energetics and charge transfer in the Ni/LaNbO4 interface from DFT calculations. *International Journal of Hydrogen Energy*, **2012**, 37, 8033-8042	6.7	6
61	Atomistic study of LaNbO4; surface properties and hydrogen adsorption. *International Journal of Hydrogen Energy*, **2012**, 37, 6674-6685	6.7	12
60	Hydrogen induced stabilization of meta-stable Mg-Ti. *Applied Physics Letters*, **2012**, 100, 111902	3.4	7
59	Theoretical analysis of oxygen vacancies in layered sodium cobaltate, Na(x)CoO(2-δ) *Journal of Physics Condensed Matter*, **2012**, 24, 475505	1.8	12

58	Crystal structure and dynamics of Mg(ND3)6Cl2. *Physical Chemistry Chemical Physics*, **2011**, 13, 7644-8	3.6	9
57	Self-diffusion in Zn4Sb3 from first-principles molecular dynamics. *Computational Materials Science*, **2011**, 50, 2663-2665	3.2	10
56	Adjustment of the decomposition path for Na2LiAlH6 by TiF3 addition. *International Journal of Hydrogen Energy*, **2011**, 36, 12279-12285	6.7	7
55	Nanovoids in thermoelectric Zn4Sb3: A possibility for nanoengineering via Zn diffusion. *Acta Materialia*, **2011**, 59, 5266-5275	8.4	32
54	Nanostructuring in Zn4Sb3 with variable starting Zn compositions. *Physica Status Solidi (A) Applications and Materials Science*, **2011**, 208, 1652-1657	1.6	22
53	XPS characterisation of in situ treated lanthanum oxide and hydroxide using tailored charge referencing and peak fitting procedures. *Journal of Electron Spectroscopy and Related Phenomena*, **2011**, 184, 399-409	1.7	323
52	Decomposition of lithium magnesium aluminum hydride. *International Journal of Hydrogen Energy*, **2011**, 36, 7602-7611	6.7	11
51	Electronic origins for sulfur interactions with palladium alloys for hydrogen-selective membranes. *Journal of Membrane Science*, **2011**, 375, 96-103	9.6	21
50	Experimental and theoretical study of electron density and structure factors in CoSb *Ultramicroscopy*, **2011**, 111, 847-53	3.1	10
49	Density functional calculations of Ti nanoclusters in the metastable Mg-Ti system. *Physical Review B* , **2010**, 82,	3.3	12
48	Role of the self-interaction error in studying chemisorption on graphene from first-principles. *Physical Review B*, **2010**, 81,	3.3	20
47	Bond analysis of phosphorus skutterudites: Elongated lanthanum electron buildup in LaFe4P12. *Computational Materials Science*, **2010**, 47, 752-757	3.2	6
46	Surface stability of potassium nitrate (KNO3) from density functional theory. *Computational Materials Science*, **2010**, 50, 356-362	3.2	6
45	X-ray photoelectron spectroscopy study of MgH2 thin films grown by reactive sputtering. *Surface and Interface Analysis*, **2010**, 42, 1140-1143	1.5	1
44	Characterization of thin and ultrathin transparent conducting oxide (TCO) films and TCO-Si interfaces with XPS, TEM and ab initio modeling. *Surface and Interface Analysis*, **2010**, 42, 874-877	1.5	6
43	Electronic structure studies of Ni-X (X: B, S, P) alloys using x-ray photoelectron spectroscopy, x-ray induced Auger electron spectroscopy and density functional theory calculations. *Journal of Physics Condensed Matter*, **2009**, 21, 245503	1.8	12
42	Viable storage of hydrogen in materials with off-board recharging using high-temperature electrolysis. *International Journal of Hydrogen Energy*, **2009**, 34, 2679-2683	6.7	6
41	Surfaces and Clusters of Mg(NH2)2 Studied by Density Functional Theory Calculations. *Journal of Physical Chemistry C*, **2009**, 113, 21648-21656	3.8	3

40	Understanding adsorption of hydrogen atoms on graphene. *Journal of Chemical Physics*, **2009**, 130, 054704	3.9	277
39	The crystal structure of LiMgAlD6 from combined neutron and synchrotron X-ray powder diffraction. *Journal of Alloys and Compounds*, **2008**, 460, 64-68	5.7	16
38	Thermodynamic modeling of the NaAlTiH system and Ti dissolution in sodium alanates. *Calphad: Computer Coupling of Phase Diagrams and Thermochemistry*, **2008**, 32, 624-636	1.9	13
37	Experimental studies of AlD3 and AlD3versus first-principles modelling of the alane isomorphs. *Journal of Materials Chemistry*, **2008**, 18, 2361		32
36	Density Functional Theory Study of the TiH2 Interaction with a NaAlH4 Cluster. *Journal of Physical Chemistry C*, **2008**, 112, 15759-15764	3.8	20
35	New filled P-based skutteruditesromising materials for thermoelectricity?. *New Journal of Physics*, **2008**, 10, 053004	2.9	6
34	Highly destabilized Mg-Ti-Ni-H system investigated by density functional theory and hydrogenography. *Physical Review B*, **2008**, 77,	3.3	32
33	Reversed surface segregation in palladium-silver alloys due to hydrogen adsorption. *Surface Science* , **2008**, 602, 2840-2844	1.8	72
32	Comparison of the electronic structure of a thermoelectric skutterudite before and after adding rattlers: an electron energy loss study. *Micron*, **2008**, 39, 685-9	2.3	4
31	NaAlH4 Clusters with Two Titanium Atoms Added. *Journal of Physical Chemistry C*, **2007**, 111, 8206-8213	3.8	20
30	Integrated experimental-theoretical investigation of the Na-Li-Al-H system. *Inorganic Chemistry*, **2007**, 46, 1401-9	5.1	14
29	Hydrogen interactions with the PdCu ordered B2 alloy. *Journal of Alloys and Compounds*, **2007**, 446-447, 583-587	5.7	47
28	Comparison of theoretical and experimental dielectric functions: Electron energy-loss spectroscopy and density-functional calculations on skutterudites. *Physical Review B*, **2006**, 74,	3.3	25
27	Stability of Ti in NaAlH4. *Applied Physics Letters*, **2006**, 88, 161917	3.4	32
26	The crystal structure and surface energy of NaAlH4: a comparison of DFT methodologies. *Journal of Physical Chemistry B*, **2006**, 110, 622-30	3.4	38
25	The crystal structure of Zr2NiD4.5. *Acta Crystallographica Section B: Structural Science*, **2006**, 62, 972-8		2
24	A density functional theory study of Ti-doped NaAlH4 clusters. *Chemical Physics Letters*, **2006**, 426, 180-186	2.5	25
23	Modeling alkali alanates for hydrogen storage by density-functional band-structure calculations. *Journal of Materials Research*, **2005**, 20, 3199-3213	2.5	39

22	Crystal structures and electronic structures of alkali aluminohexahydrides from density functional calculations. *Journal of Alloys and Compounds*, **2005**, 404-406, 757-761	5.7	15
21	Surface segregation in palladium based alloys from density-functional calculations. *Surface Science*, **2005**, 583, 100-106	1.8	101
20	Crystal structure of Ca(AlH4)2 predicted from density-functional band-structure calculations. *Physical Review B*, **2005**, 71,	3.3	56
19	Experimental and theoretical studies of plasma resonance and the electronic structure of binary skutterudites. *Materials Research Society Symposia Proceedings*, **2005**, 886, 1		
18	Density functional calculations of Ti-enhanced NaAlH4. *Physical Review B*, **2005**, 71,	3.3	103
17	Density-functional band-structure calculations of magnesium alanate Mg(AlH4)2. *Physical Review B*, **2005**, 72,	3.3	23
16	Structure and stability of possible new alanates. *Europhysics Letters*, **2004**, 67, 607-613	1.6	39
15	Crystal structure and thermodynamic stability of the lithium alanates LiAlH4 and Li3AlH6. *Physical Review B*, **2004**, 69,	3.3	100
14	The influence of electronic structure on hydrogen absorption in palladium alloys. *Journal of Physics Condensed Matter*, **2004**, 16, 6267-6277	1.8	64
13	Density-functional band-structure calculations for La-, Y-, and Sc-filled CoP3-based skutterudite structures. *Physical Review B*, **2004**, 70,	3.3	26
12	Adsorption of Ti on LiAlH4 surfaces studied by band structure calculations. *Journal of Alloys and Compounds*, **2004**, 373, 28-32	5.7	10
11	Density functional calculations of hydrogen adsorption on palladium–silver alloy surfaces. *Journal of Chemical Physics*, **2003**, 118, 3268-3276	3.9	57
10	Periodic band calculation on low index surfaces of crystalline LiAlH4. *Journal of Alloys and Compounds*, **2003**, 356-357, 178-180	5.7	14
9	A study of a polymer-based radiative cooling system. *Solar Energy*, **2002**, 73, 403-417	6.8	77
8	Density functional calculations on hydrogen in palladium–silver alloys. *Journal of Alloys and Compounds*, **2002**, 330-332, 332-337	5.7	51
7	Adsorption energies and ordered structures of hydrogen on Pd(111) from density-functional periodic calculations. *Physical Review B*, **1998**, 58, 10890-10898	3.3	78
6	The influence of surface motion on the direct subsurface absorption of H2 on Pd(111). *Journal of Chemical Physics*, **1997**, 107, 10652-10661	3.9	36
5	Direct subsurface absorption of hydrogen on Pd(111): Quantum mechanical calculations on a new two-dimensional potential energy surface. *Journal of Chemical Physics*, **1997**, 106, 9286-9296	3.9	39

4	Direct subsurface absorption of hydrogen on Pd(111). *Journal of Chemical Physics*, **1996**, 104, 4330-4336	3.9	9
3	Model calculations on a flat-plate solar heat collector with integrated solar cells. *Solar Energy*, **1995**, 55, 453-462	6.8	249
2	A Roadmap for Transforming Research to Invent the Batteries of the Future Designed within the European Large Scale Research Initiative BATTERY 2030+. *Advanced Energy Materials*,2102785	21.8	10
1	Controlling the Electrical Properties of Reactively Sputtered High Entropy Alloy CrFeNiCoCu Films. *Journal of Electronic Materials*,1	1.9	0