Jean Claude Crivello

List of Publications by Year
in descending order

83	2,648	377584 21	214428 50
papers	citations	h-index	g-index

84	84	84	2452
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Supervised deep learning prediction of the formation enthalpy of complex phases using a DFT database: The <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline" id="d1e425" altimg="si20.svg"><mml:mrow><mml:mi>Ïƒ</mml:mi><mml:mo>â^'</mml:mo></mml:mrow></mml:math>phase as an example. Computational Materials Science, 2022, 201, 110864.	1.4	11
2	Influence of self-substitution on the thermoelectric Fe2VAl Heusler alloy. Journal of Alloys and Compounds, 2022, 920, 166037.	2.8	8
3	Thermodynamic modeling of Cr and Crâ€“H systems up to high temperatures and high pressures. International Journal of Hydrogen Energy, 2022, , .	3.8	2
4	Experimental study, first-principles calculation and thermodynamic modelling of the Crâ€“Feâ€“Nbâ€“Snâ€“Zr quinary system for application as cladding materials in nuclear reactors.. Journal of Nuclear Materials, 2021, 544, 152692.	1.3	7
5	Development of Thermokinetic Tools for Phase Transformation Studies of Zr Alloys for Both In-Service and LOCA Conditions. , 2021, , 833-854.		0
6	Modification of Lu's (2005) high pressure model for improved high pressure/high temperature extrapolations. Part I: Modeling of platinum at high pressure/high temperature. Calphad: Computer Coupling of Phase Diagrams and Thermochemistry, 2021, 74, 102304.	0.7	2
7	Modification of Lu's (2005) high pressure model for improved high pressure/high temperature extrapolations. Part II: Modeling of osmiumâ€“platinum system at high pressure/high temperature. Calphad: Computer Coupling of Phase Diagrams and Thermochemistry, 2021, 74, 102311.	0.7	2
8	What is the Enthalpy Contribution to the Stabilization of the Coâ€“Crâ€“Feâ€“Mnâ€“Ni Faced-centered Cubic Solid Solution?. Journal of Phase Equilibria and Diffusion, 2021, 42, 561-570.	0.5	4
9	Low temperature study of phase equilibria in the Coâ€“Niâ€“W ternary system: evidence of a new intermetallic phase Co3W_D0a. Journal of Alloys and Compounds, 2021, 892, 162109.	2.8	1
10	TbMgNi_{4-x}Co_xâ€“(H,D)₂ System. I: Synthesis, Hydrogenation Properties, and Crystal and Electronic Structures. Journal of Physical Chemistry C, 2020, 124, 196-204.	1.5	9
11	Materials for hydrogen-based energy storage â€“ past, recent progress and future outlook. Journal of Alloys and Compounds, 2020, 827, 153548.	2.8	518
12	Relation between the weak itinerant magnetism in A ₂Ni₇ compounds (Aâ€‰â€‰=â€‰â€‰Y, La) and their stacked crystal structures. Journal of Physics Condensed Matter, 2020, 32, 145802.	2.7	6
13	Thermodynamic modelling of the Feâ€“Snâ€“Zr system based on new experiments and first-principles calculations. Journal of Alloys and Compounds, 2020, 821, 153200.	2.8	12
14	Optimization of Criteria for an Efficient Screening of New Thermoelectric Compounds: The TiNiSi Structure-Type as a Case-Study. ACS Combinatorial Science, 2020, 22, 813-820.	3.8	6
15	On the structure and electronic properties of Fe₂V_{0.8}W_{0.2}Al thin films. Physical Chemistry Chemical Physics, 2020, 22, 22549-22554.	1.3	3
16	Correlations between stacked structures and weak itinerant magnetic properties of La2 â^' x Y x Ni7 compounds. Journal of Physics Condensed Matter, 2020, 32, 415804.	0.7	6
17	Reduced phase space of heat-carrying acoustic phonons in single-crystalline InTe. Physical Review Research, 2020, 2, .	1.3	20
18	A Principled Approach to Analyze Expressiveness and Accuracy of Graph Neural Networks. Lecture Notes in Computer Science, 2020, , 27-39.	1.0	2

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19	Pdâ€“H and Niâ€“H phase diagrams using cluster variation method and Monte Carlo simulation. Philosophical Magazine, 2019, 99, 2376-2392.	0.7	4
20	Experimental and Theoretical Investigations on the Influence of A on the Hydrogen Sorption Properties of ANiy Compounds, A = {Y, Sm, Gd}. Journal of Physical Chemistry C, 2019, 123, 23334-23341.	1.5	6
21	TiVZrNb Multi-Principal-Element Alloy: Synthesis Optimization, Structural, and Hydrogen Sorption Properties. Molecules, 2019, 24, 2799.	1.7	65
22	Magnesium based materials for hydrogen based energy storage: Past, present and future. International Journal of Hydrogen Energy, 2019, 44, 7809-7859.	3.8	460
23	Mechanosynthesis and Reversible Hydrogen Storage of Mg₂Ni and Mg₂Cu Alloys. Materials Transactions, 2019, 60, 441-449.	0.4	8
24	Fast synthesis of TiNi by mechanical alloying and its hydrogenation properties. International Journal of Hydrogen Energy, 2019, 44, 10770-10776.	3.8	25
25	Description of terminal substitutional solid solutions using the sublattice model. Calphad: Computer Coupling of Phase Diagrams and Thermochemistry, 2019, 67, 101685.	0.7	4
26	Experimental investigations and thermodynamic modelling of the Crâ€“Nbâ€“Snâ€“Zr system. Calphad: Computer Coupling of Phase Diagrams and Thermochemistry, 2019, 64, 43-54.	0.7	21
27	Atomic interactions in C15 Laves phases. Journal of Materials Science, 2019, 54, 4742-4753.	1.7	4
28	Looking for new thermoelectric materials among TMX intermetallics using high-throughput calculations. Computational Materials Science, 2019, 156, 96-103.	1.4	19
29	Y6Mg9Co2 and Y9Mg30Co2: Novel magnesium-rich compounds representing new structure types. Journal of Alloys and Compounds, 2018, 737, 613-622.	2.8	6
30	Synthesis of TiFe Hydrogen Absorbing Alloys Prepared by Mechanical Alloying and SPS Treatment. Metals, 2018, 8, 264.	1.0	11
31	Vibration analysis of hydrogen, deuterium and tritium in metals: consequences on the isotope effect. Journal of Physics Condensed Matter, 2018, 30, 335402.	0.7	12
32	Thermodynamic modeling of the Moâ€“Ni system. Calphad: Computer Coupling of Phase Diagrams and Thermochemistry, 2018, 62, 215-222.	0.7	6
33	Thermodynamic modelling of the Cr-Nb-Sn system. Calphad: Computer Coupling of Phase Diagrams and Thermochemistry, 2017, 57, 37-45.	0.7	14
34	Systematic First-Principles Study of Binary Metal Hydrides. ACS Combinatorial Science, 2017, 19, 513-523.	3.8	26
35	Electronic structure, low-temperature transport and thermodynamic properties of polymorphic Î²-As₂Te₃. RSC Advances, 2016, 6, 52048-52057.	1.7	11
36	Properties of ZrNi5 deuteride synthesized under high pressure studied by neutron diffraction and first principles calculations. International Journal of Hydrogen Energy, 2016, 41, 17408-17420.	3.8	2

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37	Order-disorder transitions in the Fe2VAl Heusler alloy. Acta Materialia, 2016, 121, 126-136.	3.8	44
38	Thermodynamic assessment of the Pd Rh Ru system using calphad and first-principles methods. Journal of Nuclear Materials, 2016, 474, 163-173.	1.3	15
39	Review of magnesium hydride-based materials: development and optimisation. Applied Physics A: Materials Science and Processing, 2016, 122, 1.	1.1	274
40	Mg-based compounds for hydrogen and energy storage. Applied Physics A: Materials Science and Processing, 2016, 122, 1.	1.1	146
41	Irregular Homogeneity Domains in Ternary Intermetallic Systems. Applied Sciences (Switzerland), 2015, 5, 1570-1589.	1.3	9
42	Structural and magnetic properties of PrCo3â^'xFex by neutron powder diffraction and electronic structure investigations. Journal of Solid State Chemistry, 2015, 230, 19-25.	1.4	5
43	ZenGen, a tool to generate ordered configurations for systematic first-principles calculations: The Crâ€“Moâ€“Niâ€“Re system as a case study. Calphad: Computer Coupling of Phase Diagrams and Thermochemistry, 2015, 51, 233-240.	0.7	39
44	First principles calculations of (La,Mg)2Ni7 hydrides. Journal of Alloys and Compounds, 2015, 645, S5-S8.	2.8	13
45	Polymorphism in Thermoelectric As₂Te₃. Inorganic Chemistry, 2015, 54, 9936-9947.	1.9	25
46	Thermodynamic Modeling of the Niâ€“H System. Journal of Physical Chemistry C, 2015, 119, 24546-24557.	1.5	6
47	Structure and chemical bonding in MgNi2H3 from combined high resolution synchrotron and neutron diffraction studies and ab initio electronic structure calculations. Acta Materialia, 2015, 98, 416-422.	3.8	13
48	Hydrogen sorption properties of Pdâ€“Co nanoalloys embedded into mesoporous carbons. Nanoscale, 2015, 7, 15469-15476.	2.8	19
49	Experimental study and thermodynamic description of the erbiumâ€“hydrogenâ€“zirconium ternary system. Journal of Nuclear Materials, 2015, 456, 7-16.	1.3	1
50	Hydrogen-assisted phase transition in a trihydride MgNi2H3 synthesized at high H2 pressures: Thermodynamics, crystallographic and electronic structures. Acta Materialia, 2015, 82, 316-327.	3.8	24
51	Experimental and computed phase diagrams of the Feâ€“Re system. Journal of Physics Condensed Matter, 2014, 26, 485402.	0.7	6
52	First-principles-based phase diagrams and thermodynamic properties of TCP phases in Reâ€“X systems (X=Ta, V, W). Computational Materials Science, 2014, 81, 433-445.	1.4	32
53	Modeling of metal hydride battery anodes at high discharge current densities and constant discharge currents. Electrochimica Acta, 2014, 147, 73-81.	2.6	13
54	Phase stability in the ternary Reâ€“Wâ€“Zr system. Acta Materialia, 2014, 70, 56-65.	3.8	8

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55	Electronic and structural influence of Ni by Pd substitution on the hydrogenation properties of TiNi. Journal of Solid State Chemistry, 2013, 198, 475-484.	1.4	14
56	Structural stability of ternary C22â€“Zr6X2Co (X=Al, Ga, Sn, As, Sb, Bi, Te) and C22â€“Zr6Sn2Tâ€² (Tâ€²=Fe, Co, Ni,) Tj ETQq0 0 0 rgBT	1.4	7
57	CALPHAD description of the Moâ€“Re system focused on the sigma phase modeling. Calphad: Computer Coupling of Phase Diagrams and Thermochemistry, 2013, 43, 18-31.	0.7	41
58	Study of the magnetic and electronic properties of nanocrystalline PrCo3by neutron powder diffraction and density functional theory. Journal of Physics Condensed Matter, 2013, 25, 116001.	0.7	13
59	Structural and magnetic properties of nanocrystalline PrCo3â^'xFex. Journal of Magnetism and Magnetic Materials, 2013, 340, 10-15.	1.0	13
60	Ï‡ and Ïƒ Phases in Binary Rheniumâ€“Transition Metal Systems: a Systematic First-Principles Investigation. Inorganic Chemistry, 2013, 52, 3674-3686.	1.9	31
61	Modelling the sigma phase. MATEC Web of Conferences, 2013, 3, 01076.	0.1	0
62	Magnetic and structural properties of nanocrystalline PrCo3. IOP Conference Series: Materials Science and Engineering, 2012, 28, 012048.	0.3	5
63	Comparison of the Site Occupancies Determined by Combined Rietveld Refinement and Density Functional Theory Calculations: Example of the Ternary Moâ€“Niâ€“Re Ïƒ Phase. Inorganic Chemistry, 2012, 51, 3071-3078.	1.9	30
64	CO2 hydrogenation on a metal hydride surface. Physical Chemistry Chemical Physics, 2012, 14, 5518.	1.3	37
65	Non-Stoichiometry and Calphad Modeling of Frank-Kasper Phases. Applied Sciences (Switzerland), 2012, 2, 669-681.	1.3	23
66	Stability of erbium hydrides studied by DFT calculations. International Journal of Hydrogen Energy, 2012, 37, 4246-4253.	3.8	12
67	Structural Stability of AB_y Phases in the (La,Mg)â€“Ni System Obtained by Density Functional Theory Calculations. Journal of Physical Chemistry C, 2011, 115, 25470-25478.	1.5	75
68	Magnetic and structural properties of nanocrystalline PrCo₃. Journal of Physics: Conference Series, 2011, 303, 012028.	0.3	9
69	Density functional study of<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow><mml:mtext>Li</mml:mtext></mml:mrow><mml:mn>4</mml:mn></mml:msub> xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow><mml:mtext>Li</mml:mtext></mml:mrow><mml:mrow><mml:mn>1.5</mml:mn> Physical Review B, 2010, 81, .	1.1	16
70	First principles calculations of the Ïƒ and Ï‡ phases in the Moâ€“Re and Wâ€“Re systems. Journal of Physics Condensed Matter, 2010, 22, 035402.	0.7	31
71	Ab initio ternary -phase diagram: The Crâ€“Moâ€“Re system. Calphad: Computer Coupling of Phase Diagrams and Thermochemistry, 2010, 34, 487-494.	0.7	21
72	Improvement of Mgâ€“Al alloys for hydrogen storage applications. International Journal of Hydrogen Energy, 2009, 34, 1937-1943.	3.8	72

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73	Thermal and Magnetic Properties of Mechanically Alloyed fcc Cu-Fe Supersaturated Solid Solutions. Materials Transactions, 2008, 49, 527-531.	0.4	17
74	Synthesis of Mg-Al Alloys by Bulk Mechanical Alloying (BMA) and Their Hydrogen Solubility. Materials Transactions, 2008, 49, 2679-2685.	0.4	2
75	Development of New Transparent Conductive Material of Mg(OH)2-C. E-Journal of Surface Science and Nanotechnology, 2008, 6, 15-16.	0.1	7
76	Hydrogen absorption properties of the Î³-Mg17Al12 phase. Journal of Advanced Science, 2008, 19, 88-96.	0.1	3
77	Synthesis of Mg-Al Alloys by Bulk Mechanical Alloying (BMA) and Their Hydrogen Solubility. Nippon Kinzoku Gakkaishi/Journal of the Japan Institute of Metals, 2007, 71, 592-597.	0.2	5
78	Hydrogen absorption properties of the -Mg17Al12 phase and its Al-richer domain. Journal of Alloys and Compounds, 2007, 446-447, 157-161.	2.8	68
79	Limits of the Mgâ€“Al Î³-phase range by ball-milling. Intermetallics, 2007, 15, 1432-1437.	1.8	48
80	Hydrogen Storage Intermetallic Compounds: First Principles Investigations of Properties Relevant to Applications. Materials Science Forum, 2005, 475-479, 2489-2496.	0.3	0
81	Relationship between compressibility and hydrogen absorption in some Haucke compounds. Journal of Alloys and Compounds, 2005, 404-406, 565-569.	2.8	8
82	Magnetic properties of Crâ€“CrH and YFe2â€“YFe2H4. Journal of Alloys and Compounds, 2005, 404-406, 150-154.	2.8	6
83	Electronic properties of LaNi4.75Sn0.25, LaNi4.5M0.5 (M=Si, Ge, Sn), LaNi4.5Sn0.5H5. Journal of Alloys and Compounds, 2003, 356-357, 151-155.	2.8	19