

Luis E Gonzalez

List of Publications by Year in descending order

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218677

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122
all docs

122
docs citations

122
times ranked

865
citing authors

#	ARTICLE	IF	CITATIONS
1	First principles determination of static, dynamic and electronic properties of some liquid 4d transition metals near melting. International Journal of Refractory Metals and Hard Materials, 2022, 107, 105898.	3.8	2
2	Static structure, collective dynamics and transport coefficients in the liquid Li-Pb alloy. An ab initio molecular dynamics study. Journal of Molecular Liquids, 2021, 344, 117775.	4.9	4
3	Deuterium addition to liquid Li-Sn alloys: implications for plasma-facing applications. Nuclear Fusion, 2020, 60, 016025.	3.5	2
4	Depth-dependent dynamics of liquid metal surfaces with first principles simulations. Acta Materialia, 2020, 198, 281-289.	7.9	3
5	Neutron Brillouin scattering and <i>ab initio</i> simulation study of the collective dynamics of liquid silver. Physical Review B, 2020, 102, .	3.2	13
6	An Efficient Deep Learning Scheme To Predict the Electronic Structure of Materials and Molecules: The Example of Graphene-Derived Allotropes. Journal of Physical Chemistry A, 2020, 124, 9496-9502.	2.5	12
7	Properties of bulk liquid Pd and Pt and their free liquid surface studied with first principles techniques. Modelling and Simulation in Materials Science and Engineering, 2020, 28, 045002.	2.0	0
8	Structure and dynamics of the liquid 3d transition metals near melting. An <i>ab initio</i> study. Journal of Physics Condensed Matter, 2020, 32, 214005.	1.8	6
9	First principles determination of some static and dynamic properties of the liquid 3d transition metals near melting. Condensed Matter Physics, 2020, 23, 23606.	0.7	5
10	First principles study of liquid uranium at temperatures up to 2050 K. Journal of Physics Condensed Matter, 2020, 32, 304001.	1.8	1
11	Properties of fusion-relevant liquid Li-Sn alloys: An ab initio molecular-dynamics study. Nuclear Materials and Energy, 2019, 18, 326-330.	1.3	2
12	Orbital-free density functional theory for materials research. Journal of Materials Research, 2018, 33, 777-795.	2.6	109
13	Orbital-free density functional theory simulation of collective dynamics coupling in liquid Sn. Journal of Chemical Physics, 2018, 149, 094504.	3.0	16
14	<i>Ab initio</i> study of several static and dynamic properties of bulk liquid Ni near melting. Journal of Chemical Physics, 2017, 146, 034501.	3.0	16
15	Local order and dynamic properties of liquid Ag-Sn alloys by ab initio molecular dynamics. Journal of Non-Crystalline Solids, 2017, 473, 179-187.	3.1	2
16	First principles determination of static, dynamic and electronic properties of liquid Ti near melting. Computational Materials Science, 2017, 139, 243-251.	3.0	14
17	Globally-Optimized Local Pseudopotentials for (Orbital-Free) Density Functional Theory Simulations of Liquids and Solids. Journal of Chemical Theory and Computation, 2017, 13, 3684-3695.	5.3	18
18	Longitudinal, transverse, and single-particle dynamics in liquid Zn: <i>Ab initio</i> study and theoretical analysis. Physical Review B, 2017, 95, .	3.2	26

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19	Ab-initio study of several static and dynamic properties of liquid palladium and platinum. EPJ Web of Conferences, 2017, 151, 03002.	0.3	1
20	Orbital-free ab initio molecular dynamics study of the static structure and dynamic properties of the free liquid surface of Sn. EPJ Web of Conferences, 2017, 151, 03003.	0.3	2
21	Ab initio study of intrinsic profiles of liquid metals and their reflectivity. EPJ Web of Conferences, 2017, 151, 05002.	0.3	0
22	Dynamic properties of liquid Ni revisited. EPJ Web of Conferences, 2017, 151, 02003.	0.3	0
23	Structure and dynamics of liquid Zn: an analysis of ab-initio simulations. EPJ Web of Conferences, 2017, 151, 03004.	0.3	1
24	Orbital free ab initio study of static and dynamic properties of some liquid transition metals. EPJ Web of Conferences, 2017, 151, 03001.	0.3	2
25	An <i>ab initio</i> study of the structure and atomic transport in bulk liquid Ag and its liquid-vapor interface. Physics of Fluids, 2016, 28, .	4.0	9
26	Structure and dynamics of high-pressure Na close to the melting line: An <i>ab initio</i> molecular dynamics study. Physical Review B, 2016, 94, .	3.2	16
27	Pressure-induced changes in structural and dynamic properties of liquid Fe close to the melting line. An <i>ab initio</i> study. Journal of Physics Condensed Matter, 2016, 28, 075101.	1.8	18
28	<i>Ab initio</i> study of the structure and dynamics of bulk liquid Fe. Physical Review B, 2015, 92, .	3.2	31
29	Melting of sodium under high pressure. An ab-initio study. AIP Conference Proceedings, 2015, , .	0.4	2
30	Liquid Be, Ca and Ba. An orbital-free ab-initio molecular dynamics study. AIP Conference Proceedings, 2015, , .	0.4	0
31	Orbital free <i>ab initio</i> simulations of liquid alkaline earth metals: from pseudopotential construction to structural and dynamic properties. Journal of Physics Condensed Matter, 2014, 26, 465102.	1.8	13
32	Static and dynamic properties of liquid Zn, Cd and Hg divalent metals: An orbital free ab initio molecular dynamics study. Journal of Non-Crystalline Solids, 2014, 406, 45-53.	3.1	7
33	An <i>ab initio</i> study of the structure and dynamics of bulk liquid Cd and its liquid-vapor interface. Journal of Physics Condensed Matter, 2013, 25, 065102.	1.8	13
34	Static structure, microscopic dynamics and electronic properties of the liquid Bi-Li alloy. An <i>ab initio</i> molecular dynamics study. Modelling and Simulation in Materials Science and Engineering, 2013, 21, 075006.	2.0	7
35	<i>Ab initio</i> molecular dynamics study of the free surface of liquid Hg. Physical Review B, 2013, 87, .	3.2	7
36	An Orbital Free <i>ab initio</i> Method: Applications to Liquid Metals and Clusters. Recent Advances in Computational, 2013, , 55-145.	0.8	5

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37	Orbital free ab initio molecular dynamics simulation study of some static and dynamic properties of liquid noble metals. <i>Condensed Matter Physics</i> , 2012, 15, 33604.	0.7	11
38	Orbital free ab initio simulation of surface freezing in a dilute Ga-Tl alloy. <i>European Physical Journal: Special Topics</i> , 2011, 196, 15-26.	2.6	0
39	Expanded fluid mercury in the metal-nonmetal transition range. An ab-initio MD study. <i>European Physical Journal: Special Topics</i> , 2011, 196, 27-34.	2.6	4
40	An investigation of the local structure and dynamic properties of undercooled liquid silicon using the orbital-free ab-initio molecular dynamics method. <i>European Physical Journal: Special Topics</i> , 2011, 196, 45-52.	2.6	2
41	Transverse excitations in liquid Ga. <i>European Physical Journal: Special Topics</i> , 2011, 196, 85-93.	2.6	19
42	Static structure, microscopic dynamics and electronic properties of the liquid Bi-Pb alloy. An ab initio molecular dynamics study. <i>Journal of Nuclear Materials</i> , 2011, 411, 163-170.	2.7	18
43	Static, dynamic and electronic properties of expanded fluid mercury in the metal-nonmetal transition range. An ab initio study. <i>Journal of Physics Condensed Matter</i> , 2011, 23, 375105.	1.8	19
44	Ab initio molecular dynamics study of the static, dynamic, and electronic properties of liquid Bi near melting using real-space pseudopotentials. <i>Physical Review B</i> , 2010, 81, .	3.2	35
45	Investigation of fivefold symmetry at the liquid Pb/Si(001) interface: An ab initio molecular dynamics study. <i>Physical Review B</i> , 2010, 82, .	3.2	2
46	First-principles study of the layering at the free liquid Sn surface. <i>Physical Review B</i> , 2009, 80, .	3.2	9
47	Structural and dynamical properties of liquid Mg. An orbital-free molecular dynamics study. <i>Journal of Physics Condensed Matter</i> , 2009, 21, 115106.	1.8	23
48	Structure and motion at the liquid-vapor interface of some interalkali binary alloys: An orbital-free ab initio study. <i>Journal of Chemical Physics</i> , 2009, 130, 114703.	3.0	9
49	Computer simulation calculations of the free liquid surface of mercury. <i>Physical Review B</i> , 2009, 79, .	3.2	9
50	Ab initio molecular dynamics study of the static, dynamic, and electronic properties of liquid mercury at room temperature. <i>Journal of Chemical Physics</i> , 2009, 130, 194505.	3.0	27
51	Transverse Acoustic Excitations in Liquid Ga. <i>Physical Review Letters</i> , 2009, 102, 105502.	7.8	131
52	Structural, dynamic, and electronic properties of liquid tin: An ab initio molecular dynamics study. <i>Journal of Chemical Physics</i> , 2008, 129, 194506.	3.0	35
53	On the behavior of single-particle dynamic properties of liquid Hg and other metals. <i>Journal of Chemical Physics</i> , 2008, 129, 171103.	3.0	4
54	Structure of the liquid-vapor interfaces of Ga, In and the eutectic Ga-In alloy: an ab initio study. <i>Journal of Physics Condensed Matter</i> , 2008, 20, 114118.	1.8	13

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55	Covalentlike electronic effects in metallic liquids using an orbital-free ab initio method. <i>Physical Review B</i> , 2008, 77, .	3.2	10
56	Structure and dynamics of bulk liquid Ga and the liquid-vapor interface: An ab initio study. <i>Physical Review B</i> , 2008, 77, .	3.2	31
57	Orbital-free ab-initio study of the structure of liquid Al on a model fcc metallic wall: the influence of surface orientation.. <i>Journal of Physics: Conference Series</i> , 2008, 98, 062024.	0.4	5
58	Microscopic dynamics in liquid binary alloys: orbital-free ab-initio molecular dynamics studies. <i>Condensed Matter Physics</i> , 2008, 11, 155.	0.7	7
59	Atomic clustering in liquid Al ₃ Li: An orbital free ab initio study. <i>Journal of Non-Crystalline Solids</i> , 2007, 353, 3528-3531.	3.1	0
60	Liquid-vapor interface in the Li-Na liquid alloy. An ab initio molecular dynamics study. <i>Journal of Non-Crystalline Solids</i> , 2007, 353, 3560-3564.	3.1	3
61	Surface structure in simple liquid metals. A first principles simulation. <i>Journal of Non-Crystalline Solids</i> , 2007, 353, 3555-3559.	3.1	3
62	Ab initio molecular dynamics simulations of the static, dynamic, and electronic properties of liquid Pb using real-space pseudopotentials. <i>Physical Review B</i> , 2007, 76, .	3.2	34
63	Intrinsic structure of the free liquid surface of an alkali metal. <i>Physical Review B</i> , 2006, 74, .	3.2	18
64	Surface structure in simple liquid metals: An orbital-free first-principles study. <i>Physical Review B</i> , 2006, 74, .	3.2	29
65	Ab initio study of the atomic motion in liquid metal surfaces: comparison with Lennard-Jones systems. <i>Journal of Physics Condensed Matter</i> , 2006, 18, 11021-11030.	1.8	6
66	Model development and analysis of temperature-dependent lithium sputtering and sputtered Li+ transport for tokamak plasma-facing applications. <i>Journal of Nuclear Materials</i> , 2005, 337-339, 94-98.	2.7	11
67	Interplay between the ionic and electronic density profiles in liquid metal surfaces. <i>Journal of Chemical Physics</i> , 2005, 123, 201101.	3.0	17
68	Liquid-Vapor Interface in Liquid Binary Alloys: An Ab Initio Molecular Dynamics Study. <i>Physical Review Letters</i> , 2005, 94, 077801.	7.8	30
69	Collective modes in liquid binary alloys. An ab initio molecular dynamics study of the LiMg and LiBa alloys. <i>Journal of Physics Condensed Matter</i> , 2005, 17, 1429-1456.	1.8	12
70	Viscoelastic model for the dynamic structure factors of binary systems. <i>Physical Review E</i> , 2004, 70, 041201.	2.1	21
71	Microscopic dynamics in the liquid Li-Na alloy: An ab initio molecular dynamics study. <i>Physical Review E</i> , 2004, 69, 031205.	2.1	38
72	Thermal Properties of Impurity-Doped Clusters: Orbital-Free Molecular Dynamics Simulations of the Meltinglike Transition in Li ₁ Na ₅₄ and Cs ₁ Na ₅₄ . <i>Journal of Physical Chemistry B</i> , 2004, 108, 11722-11731.	2.6	44

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73	Surface Structure of Liquid Li and Na: An ab initio Molecular Dynamics Study. Physical Review Letters, 2004, 92, 085501.	7.8	46
74	Structure and Dynamics of Molten AgCl. The Inclusion of Induced Polarization. Journal of Physical Chemistry B, 2003, 107, 282-290.	2.6	36
75	Collective ionic dynamics in the liquid Na-Cs alloy: An ab initio molecular dynamics study. Physical Review E, 2003, 67, 041204.	2.1	30
76	Dynamic structure in a molten binary alloy by ab initio molecular dynamics: Crossover from hydrodynamics to the microscopic regime. Europhysics Letters, 2003, 62, 42-48.	2.0	9
77	Dynamical properties of liquid Al near melting: An orbital-free molecular dynamics study. Physical Review B, 2002, 65, .	3.2	86
78	Polarization effects in liquid binary alloys. Journal of Non-Crystalline Solids, 2002, 312-314, 85-89.	3.1	1
79	Atomic dynamics in simple liquid metals and alloys. Journal of Non-Crystalline Solids, 2002, 312-314, 110-120.	3.1	14
80	Density fluctuations in the liquid Na-Cs alloy. Journal of Non-Crystalline Solids, 2002, 312-314, 148-152.	3.1	1
81	Atomic dynamics in liquid Rb and Cs. Journal of Non-Crystalline Solids, 2002, 312-314, 158-162.	3.1	3
82	Modelling the structure factors and pair distribution functions of amorphous germanium, silicon and carbon. Physica B: Condensed Matter, 2002, 324, 292-304.	2.7	4
83	The bridge functions of molten salts. Journal of Chemical Physics, 2001, 115, 4676-4680.	3.0	4
84	Pseudopotentials for the calculation of dynamic properties of liquids. Journal of Physics Condensed Matter, 2001, 13, 7801-7825.	1.8	26
85	Polarization effects in liquid metals and charge stabilized colloidal dispersions. Molecular Physics, 2001, 99, 875-882.	1.7	11
86	Orbital free ab initio molecular dynamics study of liquid Al near melting. Journal of Chemical Physics, 2001, 115, 2373-2376.	3.0	48
87	A molecular dynamics study of the transport coefficients of liquid transition and noble metals using effective pair potentials obtained from the embedded atom model. Journal of Chemical Physics, 2000, 113, 10410-10411.	3.0	12
88	Density fluctuations and single-particle dynamics in liquid lithium. Physical Review B, 2000, 62, 12095-12106.	3.2	34
89	Dynamical properties of liquid lithium above the melting point. Physical Review B, 1999, 60, 10094-10106.	3.2	34
90	Orbital free ab initio molecular dynamics study of expanded liquid Cs. Journal of Non-Crystalline Solids, 1999, 250-252, 163-167.	3.1	16

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91	A theoretical and computer simulation study of the static structure and thermodynamic properties of liquid transition metals using the embedded atom model. Journal of Non-Crystalline Solids, 1999, 250-252, 53-58.	3.1	22
92	Atomic dynamics in liquid lithium near melting. Journal of Non-Crystalline Solids, 1999, 250-252, 102-106.	3.1	4
93	On the dynamical properties of the liquid Li-Na alloy. Journal of Non-Crystalline Solids, 1999, 250-252, 348-353.	3.1	9
94	Static structure and dynamics of the liquid Li-Na and Li-Mg alloys. Physical Review E, 1998, 58, 4747-4757.	2.1	25
95	Phase equilibria of the two-dimensional Lennard-Jones fluid: reference systems and perturbation theories. Molecular Physics, 1998, 93, 751-755.	1.7	15
96	Atomic dynamics in liquid alkali metals. A theoretical study. Lecture Notes in Physics, 1997, , 300-301.	0.7	0
97	Dynamic properties of liquid alkaline-earth metals. Physical Review E, 1997, 56, 6818-6828.	2.1	31
98	On the static dielectric function of liquid metals. , 1997, 103, 013.		4
99	Atomic Dynamics in Liquid Alkali Metals. A Theoretical Study. Lecture Notes in Physics, 1997, , 300-301.	0.7	0
100	Concentration dependence of the structure of liquid Li-Na and Li-Mg alloys. Journal of Non-Crystalline Solids, 1996, 205-207, 443-446.	3.1	3
101	Ion-electron pseudopotentials for liquid alloys with small charge-transfer effects. Journal of Non-Crystalline Solids, 1996, 205-207, 901-906.	3.1	1
102	Static dielectric function of liquid lithium. Journal of Non-Crystalline Solids, 1996, 205-207, 911-913.	3.1	0
103	Atomic dynamics in liquid lithium. Zeitschrift für Physik B-Condensed Matter, 1996, 100, 601-611.	1.1	25
104	A theoretical study of the static structure of the liquid alloy. Journal of Physics Condensed Matter, 1996, 8, 4465-4483.	1.8	10
105	Screening of an Ion in a Finite Electron Gas and its Relation to Cluster Structure. Physics and Chemistry of Liquids, 1995, 29, 23-30.	1.2	2
106	Static and dynamic structure of liquid lithium. Journal of Physics Condensed Matter, 1994, 6, 3849-3864.	1.8	9
107	Molecular dynamics and mean spherical approximation results for symmetric nonadditive hard core Yukawa mixtures. Journal of Chemical Physics, 1994, 100, 560-565.	3.0	5
108	Computer simulation study of liquid lithium at 470 and 843 K. Physical Review E, 1994, 50, 3656-3669.	2.1	89

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109	Molecular dynamics simulation of liquid lithium. <i>Journal of Physics Condensed Matter</i> , 1993, 5, 3095-3102.	1.8	36
110	A theoretical study of the static structure and thermodynamics of liquid lithium. <i>Journal of Physics Condensed Matter</i> , 1993, 5, 4283-4298.	1.8	44
111	The structure and electronic density distribution in the liquid alkali metals. <i>Journal of Physics Condensed Matter</i> , 1993, 5, 9261-9276.	1.8	11
112	Liquid structure of the alkaline-earth metals. <i>Physical Review E</i> , 1993, 47, 4120-4129.	2.1	28
113	Properties of a hard-core fluid with a Yukawa tail studied by molecular dynamics and the mean spherical approximation. <i>Journal of Chemical Physics</i> , 1992, 96, 6984-6988.	3.0	17
114	Variational modified hypernetted-chain approximation for multicomponent liquids: Formalism and application to simple-liquid binary mixtures. <i>Physical Review A</i> , 1992, 45, 3803-3812.	2.5	34
115	A study of binary hard core Yukawa mixtures by molecular dynamics and the mean spherical approximation. <i>Journal of Chemical Physics</i> , 1992, 97, 5121-5125.	3.0	14
116	Structure and thermodynamics of mixtures of hard D -dimensional spheres: Overlap volume function approach. <i>Journal of Chemical Physics</i> , 1992, 97, 5132-5141.	3.0	11
117	Liquid structure of titanium and vanadium; VMHNC calculations. <i>Journal of Physics Condensed Matter</i> , 1992, 4, 7651-7660.	1.8	27
118	Structure and thermodynamics of hard D -dimensional spheres: overlap volume function approach. <i>Molecular Physics</i> , 1991, 74, 613-627.	1.7	33
119	The pair distribution functions of the liquid alkali metals. <i>Physica B: Condensed Matter</i> , 1991, 168, 39-44.	2.7	23
120	Binary Yukawa mixtures: comments on the compressibility-energy thermodynamic inconsistency in the mean spherical approximation. <i>Molecular Physics</i> , 1990, 71, 157-168.	1.7	10
121	Thermodynamics of a Fluid of Hard D -dimensional Spheres: Percus-Yevick and Carnahan-Starling-like Results for $D = 4$ and 5 . <i>Physics and Chemistry of Liquids</i> , 1990, 22, 95-102.	1.2	14
122	Ordering potential and chemical short range order in the structure of model liquid binary alloys. <i>Journal of Non-Crystalline Solids</i> , 1990, 117-118, 132-135.	3.1	3