# Luis E Gonzalez

List of Publications by Year
in descending order

Source: https://exaly.com/author-pdf/605276/publications.pdf

Version: 2024-02-01

| | | | |
|---|---|---|---|
| 122 papers | 2,048 citations | 218677 26 h-index | 302126 39 g-index |
| 122 all docs | 122 docs citations | 122 times ranked | 865 citing authors |

| # | Article | IF | Citations |
|---|---|---|---|
| 1 | Transverse Acoustic Excitations in Liquid Ga. Physical Review Letters, 2009, 102, 105502. | 7.8 | 131 |
| 2 | Orbital-free density functional theory for materials research. Journal of Materials Research, 2018, 33, 777-795. | 2.6 | 109 |
| 3 | Computer simulation study of liquid lithium at 470 and 843 K. Physical Review E, 1994, 50, 3656-3669. | 2.1 | 89 |
| 4 | Dynamical properties of liquid Al near melting:â€, An orbital-free molecular dynamics study. Physical Review B, 2002, 65, . | 3.2 | 86 |
| 5 | Orbital free ab initio molecular dynamics study of liquid Al near melting. Journal of Chemical Physics, 2001, 115, 2373-2376. | 3.0 | 48 |
| 6 | Surface Structure of Liquid Li and Na: Anab initioMolecular Dynamics Study. Physical Review Letters, 2004, 92, 085501. | 7.8 | 46 |
| 7 | A theoretical study of the static structure and thermodynamics of liquid lithium. Journal of Physics Condensed Matter, 1993, 5, 4283-4298. | 1.8 | 44 |
| 8 | Thermal Properties of Impurity-Doped Clusters:â€‰ Orbital-Free Molecular Dynamics Simulations of the Meltinglike Transition in Li1Na54 and Cs1Na54. Journal of Physical Chemistry B, 2004, 108, 11722-11731. | 2.6 | 44 |
| 9 | Microscopic dynamics in the liquid Li-Na alloy: Anab initiomolecular dynamics study. Physical Review E, 2004, 69, 031205. | 2.1 | 38 |
| 10 | Molecular dynamics simulation of liquid lithium. Journal of Physics Condensed Matter, 1993, 5, 3095-3102. | 1.8 | 36 |
| 11 | Structure and Dynamics of Molten AgCl. The Inclusion of Induced Polarization. Journal of Physical Chemistry B, 2003, 107, 282-290. | 2.6 | 36 |
| 12 | Structural, dynamic, and electronic properties of liquid tin: An ab initio molecular dynamics study. Journal of Chemical Physics, 2008, 129, 194506. | 3.0 | 35 |
| 13 | Ab initiomolecular dynamics study of the static, dynamic, and electronic properties of liquid Bi near melting using real-space pseudopotentials. Physical Review B, 2010, 81, . | 3.2 | 35 |
| 14 | Variational modified hypernetted-chain approximation for multicomponent liquids: Formalism and application to simple-liquid binary mixtures. Physical Review A, 1992, 45, 3803-3812. | 2.5 | 34 |
| 15 | Dynamical properties of liquid lithium above the melting point. Physical Review B, 1999, 60, 10094-10106. | 3.2 | 34 |
| 16 | Density fluctuations and single-particle dynamics in liquid lithium. Physical Review B, 2000, 62, 12095-12106. | 3.2 | 34 |
| 17 | Ab initiomolecular dynamics simulations of the static, dynamic, and electronic properties of liquid Pb using real-space pseudopotentials. Physical Review B, 2007, 76, . | 3.2 | 34 |
| 18 | Structure and thermodynamics of hardD-dimensional spheres: overlap volume function approach. Molecular Physics, 1991, 74, 613-627. | 1.7 | 33 |

| # | Article | IF | Citations |
|---|---|---|---|
| 19 | Dynamic properties of liquid alkaline-earth metals. Physical Review E, 1997, 56, 6818-6828. | 2.1 | 31 |
| 20 | Structure and dynamics of bulk liquid Ga and the liquid-vapor interface: Anab initiostudy. Physical Review B, 2008, 77, . | 3.2 | 31 |
| 21 | Ab initiostudy of the structure and dynamics of bulk liquid Fe. Physical Review B, 2015, 92, . | 3.2 | 31 |
| 22 | Collective ionic dynamics in the liquid Na-Cs alloy: Anab initiomolecular dynamics study. Physical Review E, 2003, 67, 041204. | 2.1 | 30 |
| 23 | Liquid-Vapor Interface in Liquid Binary Alloys: AnAb InitioMolecular Dynamics Study. Physical Review Letters, 2005, 94, 077801. | 7.8 | 30 |
| 24 | Surface structure in simple liquid metals: An orbital-free first-principles study. Physical Review B, 2006, 74, . | 3.2 | 29 |
| 25 | Liquid structure of the alkaline-earth metals. Physical Review E, 1993, 47, 4120-4129. | 2.1 | 28 |
| 26 | Liquid structure of titanium and vanadium; VMHNC calculations. Journal of Physics Condensed Matter, 1992, 4, 7651-7660. | 1.8 | 27 |
| 27 | Ab initio molecular dynamics study of the static, dynamic, and electronic properties of liquid mercury at room temperature. Journal of Chemical Physics, 2009, 130, 194505. | 3.0 | 27 |
| 28 | Pseudopotentials for the calculation of dynamic properties of liquids. Journal of Physics Condensed Matter, 2001, 13, 7801-7825. | 1.8 | 26 |
| 29 | Longitudinal, transverse, and single-particle dynamics in liquid Zn:Ab initiostudy and theoretical analysis. Physical Review B, 2017, 95, . | 3.2 | 26 |
| 30 | Atomic dynamics in liquid lithium. Zeitschrift FÃ¼r Physik B-Condensed Matter, 1996, 100, 601-611. | 1.1 | 25 |
| 31 | Static structure and dynamics of the liquid Li-Na and Li-Mg alloys. Physical Review E, 1998, 58, 4747-4757. | 2.1 | 25 |
| 32 | The pair distribution functions of the liquid alkali metals. Physica B: Condensed Matter, 1991, 168, 39-44. | 2.7 | 23 |
| 33 | Structural and dynamical properties of liquid Mg. An orbital-free molecular dynamics study. Journal of Physics Condensed Matter, 2009, 21, 115106. | 1.8 | 23 |
| 34 | 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 |
| 35 | Viscoelastic model for the dynamic structure factors of binary systems. Physical Review E, 2004, 70, 041201. | 2.1 | 21 |
| 36 | Transverse excitations in liquid Ga. European Physical Journal: Special Topics, 2011, 196, 85-93. | 2.6 | 19 |

| # | Article | IF | Citations |
|---|---|---|---|
| 37 | Static, dynamic and electronic properties of expanded fluid mercury in the metalâ€“nonmetal transition range. Anab initiostudy. Journal of Physics Condensed Matter, 2011, 23, 375105. | 1.8 | 19 |
| 38 | Intrinsic structure of the free liquid surface of an alkali metal. Physical Review B, 2006, 74, . | 3.2 | 18 |
| 39 | Static structure, microscopic dynamics and electronic properties of the liquid Biâ€“Pb alloy. An ab initio molecular dynamics study. Journal of Nuclear Materials, 2011, 411, 163-170. | 2.7 | 18 |
| 40 | Pressure-induced changes in structural and dynamic properties of liquid Fe close to the melting line. Anab initiostudy. Journal of Physics Condensed Matter, 2016, 28, 075101. | 1.8 | 18 |
| 41 | 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 |
| 42 | Properties of a hardâ€core fluid with a Yukawa tail studied by molecular dynamics and the mean spherical approximation. Journal of Chemical Physics, 1992, 96, 6984-6988. | 3.0 | 17 |
| 43 | Interplay between the ionic and electronic density profiles in liquid metal surfaces. Journal of Chemical Physics, 2005, 123, 201101. | 3.0 | 17 |
| 44 | Orbital free ab initio molecular dynamics study of expanded liquid Cs. Journal of Non-Crystalline Solids, 1999, 250-252, 163-167. | 3.1 | 16 |
| 45 | Structure and dynamics of high-pressure Na close to the melting line: Anab initiomolecular dynamics study. Physical Review B, 2016, 94, . | 3.2 | 16 |
| 46 | Ab initio study of several static and dynamic properties of bulk liquid Ni near melting. Journal of Chemical Physics, 2017, 146, 034501. | 3.0 | 16 |
| 47 | Orbital-free density functional theory simulation of collective dynamics coupling in liquid Sn. Journal of Chemical Physics, 2018, 149, 094504. | 3.0 | 16 |
| 48 | Phase equilibria of the two-dimensional Lennard-Jones fluid: reference systems and perturbation theories. Molecular Physics, 1998, 93, 751-755. | 1.7 | 15 |
| 49 | Thermodynamics of a Fluid of Hard D-dimensional Spheres: Percus-Yevick and Carnahan-Starling-like Results for D = 4 and 5. Physics and Chemistry of Liquids, 1990, 22, 95-102. | 1.2 | 14 |
| 50 | A study of binary hard core Yukawa mixtures by molecular dynamics and the mean spherical approximation. Journal of Chemical Physics, 1992, 97, 5121-5125. | 3.0 | 14 |
| 51 | Atomic dynamics in simple liquid metals and alloys. Journal of Non-Crystalline Solids, 2002, 312-314, 110-120. | 3.1 | 14 |
| 52 | First principles determination of static, dynamic and electronic properties of liquid Ti near melting. Computational Materials Science, 2017, 139, 243-251. | 3.0 | 14 |
| 53 | Structure of the liquidâ€“vapor interfaces of Ga, In and the eutectic Gaâ€“In alloyâ€”anab initiostudy. Journal of Physics Condensed Matter, 2008, 20, 114118. | 1.8 | 13 |
| 54 | Anab initiostudy of the structure and dynamics of bulk liquid Cd and its liquidâ€“vapor interface. Journal of Physics Condensed Matter, 2013, 25, 065102. | 1.8 | 13 |

| # | Article | IF | Citations |
|---|---|---|---|
| 55 | Orbital freeab initiosimulations of liquid alkaline earth metals: from pseudopotential construction to structural and dynamic properties. Journal of Physics Condensed Matter, 2014, 26, 465102. | 1.8 | 13 |
| 56 | Neutron Brillouin scattering and ab initio simulation study of the collective dynamics of liquid silver. Physical Review B, 2020, 102, . | 3.2 | 13 |
| 57 | 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 |
| 58 | Collective modes in liquid binary alloys. Anab initiomolecular dynamics study of the LiMg and LiBa alloys. Journal of Physics Condensed Matter, 2005, 17, 1429-1456. | 1.8 | 12 |
| 59 | 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 |
| 60 | Structure and thermodynamics of mixtures of hard Dâ€dimensional spheres: Overlap volume function approach. Journal of Chemical Physics, 1992, 97, 5132-5141. | 3.0 | 11 |
| 61 | The structure and electronic density distribution in the liquid alkali metals. Journal of Physics Condensed Matter, 1993, 5, 9261-9276. | 1.8 | 11 |
| 62 | Polarization effects in liquid metals and charge stabilized colloidal dispersions. Molecular Physics, 2001, 99, 875-882. | 1.7 | 11 |
| 63 | Model development and analysis of temperature-dependent lithium sputtering and sputtered Li+ transport for tokamak plasma-facing applications. Journal of Nuclear Materials, 2005, 337-339, 94-98. | 2.7 | 11 |
| 64 | Orbital free ab initio molecular dynamics simulation study of some static and dynamic properties of liquid noble metals. Condensed Matter Physics, 2012, 15, 33604. | 0.7 | 11 |
| 65 | Binary Yukawa mixtures: comments on the compressibility-energy thermodynamic inconsistency in the mean spherical approximation. Molecular Physics, 1990, 71, 157-168. | 1.7 | 10 |
| 66 | A theoretical study of the static structure of the liquid alloy. Journal of Physics Condensed Matter, 1996, 8, 4465-4483. | 1.8 | 10 |
| 67 | Covalentlike electronic effects in metallic liquids using an orbital-freeab initiomethod. Physical Review B, 2008, 77, . | 3.2 | 10 |
| 68 | Static and dynamic structure of liquid lithium. Journal of Physics Condensed Matter, 1994, 6, 3849-3864. | 1.8 | 9 |
| 69 | On the dynamical properties of the liquid Liâ€“Na alloy. Journal of Non-Crystalline Solids, 1999, 250-252, 348-353. | 3.1 | 9 |
| 70 | Dynamic structure in a molten binary alloy byab initiomolecular dynamics: Crossover from hydrodynamics to the microscopic regime. Europhysics Letters, 2003, 62, 42-48. | 2.0 | 9 |
| 71 | First-principles study of the layering at the free liquid Sn surface. Physical Review B, 2009, 80, . | 3.2 | 9 |
| 72 | Structure and motion at the liquid-vapor interface of some interalkali binary alloys: An orbital-free ab initio study. Journal of Chemical Physics, 2009, 130, 114703. | 3.0 | 9 |

| # | Article | IF | Citations |
|---|---|---|---|
| 73 | Computer simulation calculations of the free liquid surface of mercury. Physical Review B, 2009, 79, . | 3.2 | 9 |
| 74 | An ab initio study of the structure and atomic transport in bulk liquid Ag and its liquid-vapor interface. Physics of Fluids, 2016, 28, . | 4.0 | 9 |
| 75 | Static structure, microscopic dynamics and electronic properties of the liquid Biâ€“Li alloy. Anab initiomolecular dynamics study. Modelling and Simulation in Materials Science and Engineering, 2013, 21, 075006. | 2.0 | 7 |
| 76 | Ab initiomolecular dynamics study of the free surface of liquid Hg. Physical Review B, 2013, 87, . | 3.2 | 7 |
| 77 | 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 |
| 78 | Microscopic dynamics in liquid binary alloys: orbital-free ab-initio molecular dynamics studies. Condensed Matter Physics, 2008, 11, 155. | 0.7 | 7 |
| 79 | Ab initiostudy of the atomic motion in liquid metal surfaces: comparison with Lennard-Jones systems. Journal of Physics Condensed Matter, 2006, 18, 11021-11030. | 1.8 | 6 |
| 80 | Structure and dynamics of the liquid 3d transition metals near melting. An ab initio study. Journal of Physics Condensed Matter, 2020, 32, 214005. | 1.8 | 6 |
| 81 | 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 |
| 82 | Orbital-free ab-initio study of the structure of liquid Al on a model fcc metallic wall: the influence of surface orientation.. Journal of Physics: Conference Series, 2008, 98, 062024. | 0.4 | 5 |
| 83 | An Orbital Free ab initio Method: Applications to Liquid Metals and Clusters. Recent Advances in Computational, 2013, , 55-145. | 0.8 | 5 |
| 84 | 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 |
| 85 | Atomic dynamics in liquid lithium near melting. Journal of Non-Crystalline Solids, 1999, 250-252, 102-106. | 3.1 | 4 |
| 86 | The bridge functions of molten salts. Journal of Chemical Physics, 2001, 115, 4676-4680. | 3.0 | 4 |
| 87 | 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 |
| 88 | On the behavior of single-particle dynamic properties of liquid Hg and other metals. Journal of Chemical Physics, 2008, 129, 171103. | 3.0 | 4 |
| 89 | Expanded fluid mercury in the metal-nonmetal transition range. An ab-initio MD study. European Physical Journal: Special Topics, 2011, 196, 27-34. | 2.6 | 4 |
| 90 | On the static dielectric function of liquid metals. , 1997, 103, 013. | | 4 |

| # | Article | IF | Citations |
|---|---|---|---|
| 91 | 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 |
| 92 | Ordering potential and chemical short range order in the structure of model liquid binary alloys. Journal of Non-Crystalline Solids, 1990, 117-118, 132-135. | 3.1 | 3 |
| 93 | 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 |
| 94 | Atomic dynamics in liquid Rb and Cs. Journal of Non-Crystalline Solids, 2002, 312-314, 158-162. | 3.1 | 3 |
| 95 | Liquidâ€“vapor interface in the Liâ€“Na liquid alloy. An ab initio molecular dynamics study. Journal of Non-Crystalline Solids, 2007, 353, 3560-3564. | 3.1 | 3 |
| 96 | Surface structure in simple liquid metals. A first principles simulation. Journal of Non-Crystalline Solids, 2007, 353, 3555-3559. | 3.1 | 3 |
| 97 | Depth-dependent dynamics of liquid metal surfaces with first principles simulations. Acta Materialia, 2020, 198, 281-289. | 7.9 | 3 |
| 98 | 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 |
| 99 | Investigation of fivefold symmetry at the liquid Pb/Si(001) interface: Anab initiomolecular dynamics study. Physical Review B, 2010, 82, . | 3.2 | 2 |
| 100 | An investigation of the local structure and dynamic properties of undercooled liquid silicon using the orbital-free ab-initio molecular dynamics method. European Physical Journal: Special Topics, 2011, 196, 45-52. | 2.6 | 2 |
| 101 | Melting of sodium under high pressure. An ab-initio study. AIP Conference Proceedings, 2015, , . | 0.4 | 2 |
| 102 | Local order and dynamic properties of liquid Ag -Sn1â^' alloys by ab initio molecular dynamics. Journal of Non-Crystalline Solids, 2017, 473, 179-187. | 3.1 | 2 |
| 103 | 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 |
| 104 | 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 |
| 105 | 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 |
| 106 | Deuterium addition to liquid Liâ€“Sn alloys: implications for plasma-facing applications. Nuclear Fusion, 2020, 60, 016025. | 3.5 | 2 |
| 107 | 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 |
| 108 | Ion-electron pseudopotentials for liquid alloys with small charge-transfer effects. Journal of Non-Crystalline Solids, 1996, 205-207, 901-906. | 3.1 | 1 |

| # | Article | IF | Citations |
|---|---|---|---|
| 109 | Polarization effects in liquid binary alloys. Journal of Non-Crystalline Solids, 2002, 312-314, 85-89. | 3.1 | 1 |
| 110 | Density fluctuations in the liquid Naâ€“Cs alloy.. Journal of Non-Crystalline Solids, 2002, 312-314, 148-152. | 3.1 | 1 |
| 111 | Ab-initio study of several static and dynamic properties of liquid palladium and platinum. EPJ Web of Conferences, 2017, 151, 03002. | 0.3 | 1 |
| 112 | Structure and dynamics of liquid Zn: an analysis of ab-initio simulations. EPJ Web of Conferences, 2017, 151, 03004. | 0.3 | 1 |
| 113 | First principles study of liquid uranium at temperatures up to 2050 K. Journal of Physics Condensed Matter, 2020, 32, 304001. | 1.8 | 1 |
| 114 | Static dielectric function of liquid lithium. Journal of Non-Crystalline Solids, 1996, 205-207, 911-913. | 3.1 | 0 |
| 115 | Atomic dynamics in liquid alkali metals. A theoretical study. Lecture Notes in Physics, 1997, , 300-301. | 0.7 | 0 |
| 116 | Atomic clustering in liquid Al3Li: An orbital free ab initio study. Journal of Non-Crystalline Solids, 2007, 353, 3528-3531. | 3.1 | 0 |
| 117 | Orbital free ab initio simulation of surface freezing in a dilute Ga-Tl alloy. European Physical Journal: Special Topics, 2011, 196, 15-26. | 2.6 | 0 |
| 118 | Liquid Be, Ca and Ba. An orbital-free ab-initio molecular dynamics study. AIP Conference Proceedings, 2015, , . | 0.4 | 0 |
| 119 | Ab initio study of intrinsic profiles of liquid metals and their reflectivity. EPJ Web of Conferences, 2017, 151, 05002. | 0.3 | 0 |
| 120 | Dynamic properties of liquid Ni revisited. EPJ Web of Conferences, 2017, 151, 02003. | 0.3 | 0 |
| 121 | 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 |
| 122 | Atomic Dynamics in Liquid Alkali Metals. A Theoretical Study. Lecture Notes in Physics, 1997, , 300-301. | 0.7 | 0 |