

# Aitor Bergara

## List of Publications by Year in descending order

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105  
papers

3,400  
citations

147566

31  
h-index

155451

55  
g-index

107  
all docs

107  
docs citations

107  
times ranked

2278  
citing authors

#	ARTICLE	IF	CITATIONS
1	Superconducting High Pressure Phase of Germane. Physical Review Letters, 2008, 101, 107002.	2.9	224
2	Anomalous High-Temperature Superconductivity in $\text{YH}_6$ . Advanced Materials, 2021, 33, e2006832.	11.1	196
3	Structures and Potential Superconductivity in $\text{SiH}_4$ at High Pressure: En Route to "Metallic Hydrogen". Physical Review Letters, 2006, 96, 017006.	2.9	187
4	High-pressure crystal structures and superconductivity of Stannane ( $\text{SnH}_4$ ). Proceedings of the National Academy of Sciences of the United States of America, 2010, 107, 1317-1320.	3.3	168
5	Novel Structures and Superconductivity of Silane under Pressure. Physical Review Letters, 2009, 102, 087005.	2.9	146
6	Two-Dimensional $\text{PC}_6$ with Direct Band Gap and Anisotropic Carrier Mobility. Journal of the American Chemical Society, 2019, 141, 1599-1605.	6.6	144
7	Potential high-temperature superconductivity in $\text{CaYH}_{12}$ under pressure. Physical Review B, 2019, 80, .	1.1	109
8	Gold as a 6p-Element in Dense Lithium Aurides. Journal of the American Chemical Society, 2016, 138, 4046-4052.	6.6	101
9	Predicted Pressure-Induced Superconducting Transition in Electride $\text{Li}_6\text{P}$ . Physical Review Letters, 2019, 122, 097002.	2.9	94
10	Phonon Collapse and Second-Order Phase Transition in Thermoelectric SnSe. Physical Review Letters, 2019, 122, 075901.	2.9	92
11	Exotic behavior and crystal structures of calcium under pressure. Proceedings of the National Academy of Sciences of the United States of America, 2010, 107, 7646-7651.	3.3	86
12	Anharmonic effects in atomic hydrogen: Superconductivity and lattice dynamical stability. Physical Review B, 2016, 93, .	1.1	75
13	Anharmonic Stabilization of the High-Pressure Simple Cubic Phase of Calcium. Physical Review Letters, 2011, 106, 165501.	2.9	73
14	First-Principles Simulations of Lithium Melting: Stability of the bcc Phase Close to Melting. Physical Review Letters, 2010, 104, 185701.	2.9	67
15	Prediction of high-temperature superconductivity in ternary lanthanum borohydrides. Physical Review B, 2021, 104, .	1.1	66
16	Metallic and superconducting gallane under high pressure. Physical Review B, 2011, 84, .	1.1	65
17	Crystal structure of $\text{Si}_4\text{H}_4$ at high pressure. Physical Review B, 2007, 76, .	1.1	63
18	Theoretical study of the ground-state structures and properties of niobium hydrides under pressure. Physical Review B, 2013, 88, .	1.1	63

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19	Exotic high pressure behavior of light alkali metals, lithium and sodium. European Physical Journal B, 2011, 81, 1-14.	0.6	62
20	Pressure induced metallization of Germane. Journal of Physics and Chemistry of Solids, 2006, 67, 2095-2099.	1.9	59
21	Giant anharmonicity suppresses superconductivity in $\text{AlH}_3$ at high pressure. Physical Review B, 2010, 82, .	1.1	54
22	Relativistic effects and fully spin-polarized Fermi surface at the Tl/Si(111) surface. Physical Review B, 2011, 84, .	1.1	50
23	Complexity and Fermi surface deformation in compressed lithium. Physical Review B, 2006, 74, .	1.1	43
24	Efficient computation of magnon dispersions within time-dependent density functional theory using maximally localized Wannier functions. Physical Review B, 2012, 85, .	1.1	39
25	Structural, Vibrational, and Electronic Study of $\text{As}_2\text{Te}_3$ under Compression. Journal of Physical Chemistry C, 2016, 120, 19340-19352.	1.5	37
26	Pressure-Induced Stable $\text{Li}_5\text{P}$ for High-Performance Lithium-Ion Batteries. Journal of Physical Chemistry C, 2017, 121, 21199-21205.	1.5	36
27	Strong anharmonicity and high thermoelectric efficiency in high-temperature SnS from first principles. Physical Review B, 2019, 100, .	1.1	35
28	Pairing, $\pi$ -bonding, and the role of nonlocality in a dense lithium monolayer. Physical Review B, 2000, 62, 8494-8499.	1.1	34
29	First-principles study of crystal structures and superconductivity of ternary $\text{YSH}_6$ and $\text{LaSH}_6$ at high pressures. Physical Review B, 2019, 100, .	1.1	33
30	A model for the velocity-dependent screening. Nuclear Instruments & Methods in Physics Research B, 1996, 115, 58-61.	0.6	31
31	Tight-binding models for ultracold atoms in honeycomb optical lattices. Physical Review A, 2013, 87, .	1.0	31
32	Enhanced Friedel Structure and Proton Pairing in Dense Solid Hydrogen. Physical Review Letters, 2003, 90, 035501.	2.9	30
33	Fermi surface nesting and phonon instabilities in simple cubic calcium. High Pressure Research, 2008, 28, 443-448.	0.4	30
34	Nonmetallic $\text{FeH}_6$ under High Pressure. Journal of Physical Chemistry C, 2018, 122, 12022-12028.	1.5	29
35	Anharmonic enhancement of superconductivity in metallic molecular $\text{Cmca}\sqrt{2}\sqrt{2}\sqrt{2}$ hydrogen at high pressure: a first-principles study. Journal of Physics Condensed Matter, 2016, 28, 494001.	0.7	26
36	A New Three-Dimensional Subsulfide $\text{Ir}_2\text{In}_8\text{S}$ with Dirac Semimetal Behavior. Journal of the American Chemical Society, 2019, 141, 19130-19137.	6.6	26

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37	Quadratic electronic response of a two-dimensional electron gas. <i>Physical Review B</i> , 1999, 59, 10145-10151.	1.1	25
38	Pressure induced complexity in a lithium monolayer: Ab initio calculations. <i>Physical Review B</i> , 2005, 72, .	1.1	23
39	Lindemann criterion and the anomalous melting curve of sodium. <i>Journal of Physics and Chemistry of Solids</i> , 2008, 69, 2151-2154.	1.9	23
40	LiB and its boron-deficient variants under pressure. <i>Physical Review B</i> , 2012, 86, .	1.1	23
41	Quadratic induced polarization by an external heavy charge in an electron gas. <i>Physical Review B</i> , 1997, 56, 15654-15664.	1.1	22
42	No evidence of metallic methane at high pressure. <i>High Pressure Research</i> , 2006, 26, 369-375.	0.4	21
43	Spin-Flip Transitions Induced by Time-Dependent Electric Fields in Surfaces with Strong Spin-Orbit Interaction. <i>Physical Review Letters</i> , 2012, 109, 156401.	2.9	20
44	Weyl fermions, Fermi arcs, and minority-spin carriers in ferromagnetic CoS <sub>2</sub> . <i>Science Advances</i> , 2020, 6, .	4.7	20
45	Ferromagnetic instabilities in atomically thin lithium and sodium wires. <i>International Journal of Quantum Chemistry</i> , 2003, 91, 239-244.	1.0	19
46	Superconducting boron allotropes. <i>Physical Review B</i> , 2020, 101, .	1.1	18
47	Anisotropic and High-Mobility C <sub>3</sub> S Monolayer as a Photocatalyst for Water Splitting. <i>Journal of Physical Chemistry Letters</i> , 2021, 12, 8320-8327.	2.1	18
48	Pressure induced phase transitions in TiH <sub>2</sub> . <i>Journal of Applied Physics</i> , 2013, 113, 103512.	1.1	17
49	Novel superhard boron-rich nitrides under pressure. <i>Science China Materials</i> , 2020, 63, 2358-2364.	3.5	17
50	Energy-loss rates of heavy and light charged particles in a two-dimensional electron gas. <i>Physical Review B</i> , 1997, 55, 12864-12867.	1.1	16
51	Ab initio dynamical response of metal monolayers. <i>Physical Review B</i> , 2003, 67, .	1.1	16
52	Energy loss spectra of lithium under pressure. <i>New Journal of Physics</i> , 2008, 10, 053035.	1.2	16
53	Ab initio study of superconducting hexagonal Be <sub>2</sub> Li under pressure. <i>Physical Review B</i> , 2008, 78, .	1.1	16
54	Hard and superconducting cubic boron phase via swarm-intelligence structural prediction driven by a machine-learning potential. <i>Physical Review B</i> , 2021, 103, .	1.1	16

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55	Strong variation of dielectric response and optical properties of lithium under pressure. <i>Physical Review B</i> , 2007, 75, .	1.1	15
56	Electronic collective excitations in compressed lithium from <i>ab initio</i> calculations: Importance and anisotropy of local-field effects at large momenta. <i>Physical Review B</i> , 2010, 81, .	1.1	15
57	Self-consistent tight-binding description of Dirac points moving and merging in two-dimensional optical lattices. <i>Physical Review A</i> , 2013, 88, .	1.0	15
58	Strong Electron-Phonon and Band Structure Effects in the Optical Properties of High Pressure Metallic Hydrogen. <i>Physical Review Letters</i> , 2018, 120, 057402.	2.9	15
59	Plasmon excitation by charged particles interacting with metal surfaces. <i>Physics Letters, Section A: General, Atomic and Solid State Physics</i> , 1999, 256, 405-410.	0.9	14
60	Phase diagrams and electronic properties of B-S and H-B-S systems under high pressure. <i>Physical Review B</i> , 2019, 100, .	1.1	14
61	Anisotropic PC <sub>6</sub> N Monolayer with Wide Band Gap and Ultrahigh Carrier Mobility. <i>Journal of Physical Chemistry C</i> , 2020, 124, 4330-4337.	1.5	14
62	Pressure-induced superconductivity in Li-Te electrides. <i>Physical Review B</i> , 2021, 104, .	1.1	14
63	Spin-flip transitions and departure from the Rashba model in the Au(111) surface. <i>Physical Review B</i> , 2013, 88, .	1.1	12
64	Prediction of superconductivity in pressure-induced new silicon boride phases. <i>Physical Review B</i> , 2020, 101, .	1.1	12
65	Nonlinear effects on charged particle interactions in matter. <i>Nuclear Instruments &amp; Methods in Physics Research B</i> , 1995, 99, 187-191.	0.6	11
66	The Subchalcogenides Ir <sub>2</sub> In <sub>8</sub> Q (Q = S, Se, Te): Dirac Semimetal Candidates with Re-entrant Structural Modulation. <i>Journal of the American Chemical Society</i> , 2020, 142, 6312-6323.	6.6	11
67	Ba with Unusual Oxidation States in Ba Chalcogenides under Pressure. <i>Journal of Physical Chemistry Letters</i> , 2021, 12, 4203-4210.	2.1	11
68	Breakdown of the Peierls substitution for the Haldane model with ultracold atoms. <i>Physical Review A</i> , 2014, 90, .	1.0	10
69	Wide Band Gap P <sub>3</sub> S Monolayer with Anisotropic and Ultrahigh Carrier Mobility. <i>Journal of Physical Chemistry Letters</i> , 2021, 12, 8481-8488.	2.1	10
70	Spectral and optical properties of Ag <sub>3</sub> Au(Se <sub>2</sub> , Te <sub>2</sub> ) and dark matter detection. <i>JPhys Materials</i> , 2020, 3, 014001.	1.8	9
71	Achieving high hydrogen evolution reaction activity of a Mo <sub>2</sub> C monolayer. <i>Physical Chemistry Chemical Physics</i> , 2020, 22, 26189-26199.	1.3	9
72	Nonlinear wake in the random-phase-approximation. <i>Nuclear Instruments &amp; Methods in Physics Research B</i> , 1995, 96, 604-609.	0.6	8

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73	Structural and Superconducting Properties of Tungsten Hydrides Under High Pressure. <i>Frontiers in Physics</i> , 2018, 6, .	1.0	8
74	Superconducting $\text{LaP}_2\text{H}_2$ with graphenelike phosphorus layers. <i>Physical Review B</i> , 2022, 105, .	1.1	8
75	Nonlinear quantum hydrodynamical model of the electron gas. <i>Nuclear Instruments &amp; Methods in Physics Research B</i> , 1996, 115, 70-74.	0.6	7
76	$\hat{I}^2$ : Pressure-induced three-dimensional Dirac semimetal with ultralow room-pressure lattice thermal conductivity. <i>Physical Review B</i> , 2021, 104, .	1.1	7
77	Cubic Hall viscosity in three-dimensional topological semimetals. <i>Physical Review Research</i> , 2021, 3, .	1.3	7
78	Hydrodynamic approximation for the nonlinear response of a metal surface. <i>Physical Review B</i> , 1999, 60, 16176-16185.	1.1	6
79	Optical properties of calcium under pressure from first-principles calculations. <i>Physical Review B</i> , 2012, 86, .	1.1	6
80	Ab initio analysis of plasmon dispersion in sodium under pressure. <i>Physical Review B</i> , 2014, 89, .	1.1	6
81	Nesting Induced Peierls-Type Instability for Compressed Li <sub>16</sub> . <i>Journal of the Physical Society of Japan</i> , 2007, 76, 21-22.	0.7	5
82	Kohn anomalies and enhanced superconductivity in simple systems under pressure: Insights from the nearly free electron model. <i>Journal of Physics and Chemistry of Solids</i> , 2010, 71, 1159-1164.	1.9	5
83	Undamped low-energy plasmon in $\text{AlH}_3$ at high pressure. <i>Physical Review B</i> , 2010, 82, .		
84	Anharmonicity in aluminum hydride at high pressures. <i>High Pressure Research</i> , 2011, 31, 30-34.	0.4	5
85	Isotope effect in the superconducting high-pressure simple cubic phase of calcium from first principles. <i>Journal of Applied Physics</i> , 2012, 111, 112604.	1.1	5
86	Ab initio analysis of the topological phase diagram of the Haldane model. <i>Physical Review B</i> , 2015, 92, .	1.1	5
87	An epilepsy-causing mutation leads to co-translational misfolding of the Kv7.2 channel. <i>BMC Biology</i> , 2021, 19, 109.	1.7	5
88	Nonlinear corrections to the image potential of charged particles moving parallel to a metal surface. <i>Nuclear Instruments &amp; Methods in Physics Research B</i> , 1998, 135, 97-102.	0.6	4
89	Enhanced Anharmonicity Under Pressure. <i>Journal of Physics: Conference Series</i> , 2012, 377, 012060.	0.3	4
90	Anharmonicity and the isotope effect in superconducting lithium at high pressures: A first-principles approach. <i>Physical Review B</i> , 2017, 96, .	1.1	4

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91	Phase transitions of alkaline-earth metal sulfides under pressure. <i>Materials Research Express</i> , 2021, 8, 065902.	0.8	4
92	Theoretical study of topological properties of ferromagnetic pyrite $\text{CoS}_2$ . <i>Journal Physics D: Applied Physics</i> , 2022, 55, 304004.	1.3	4
93	Dynamical response function of a compressed lithium monolayer. <i>Surface Science</i> , 2006, 600, 3856-3859.	0.8	3
94	Fermi surface deformation in lithium under high pressure. <i>High Pressure Research</i> , 2006, 26, 461-465.	0.4	3
95	High pressure phases of different tetraboranes. <i>High Pressure Research</i> , 2014, 34, 59-69.	0.4	3
96	Do calmodulin binding IQ motifs have built-in capping domains?. <i>Protein Science</i> , 2021, 30, 2029-2041.	3.1	3
97	On the validity of perturbative treatments for the static screening in a charged-boson gas. <i>Journal of Physics Condensed Matter</i> , 1999, 11, 3943-3949.	0.7	2
98	Ab initio superconducting temperature of $\text{BaSi}_2$ at ambient pressure. <i>Journal of Physics: Conference Series</i> , 2010, 215, 012109.	0.3	2
99	Anomalous static electronic screening in compressed lithium. <i>Journal of Physics: Conference Series</i> , 2008, 121, 012007.	0.3	1
100	Structural characterization of slightly boron-deficient LiB, $\text{LiB}_{0.9}$ and $\text{LiB}_{0.8}$ , under pressure. <i>Journal of Physics Condensed Matter</i> , 2014, 26, 475402.	0.7	1
101	Semiconducting $\text{MnB}_5$ monolayer as a potential photovoltaic material. <i>Journal of Physics Condensed Matter</i> , 2021, 33, 175702.	0.7	1
102	Dynamical stability of face centered cubic lithium at 25 GPa. , 0, , .		1
103	Quadratic Response Solutions for Different Nonlinear Approaches of Static Screening: A Comparative Study. , 2002, , 657-661.		0
104	Publisher's Note: Spin-flip transitions and departure from the Rashba model in the Au(111) surface [ <i>Phys. Rev. B</i> 88, 125404 (2013)]. <i>Physical Review B</i> , 2013, 88, .	1.1	0
105	Plasmons in Li under compression. <i>Journal of Physics Condensed Matter</i> , 2019, 31, 185501.	0.7	0