

# Aitor Bergara

## List of Publications by Citations

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The third column is the impact factor (IF) of the journal, and the fourth column is the number of citations of the article.

99  
papers

2,500  
citations

27  
h-index

47  
g-index

107  
ext. papers

2,994  
ext. citations

4.4  
avg, IF

5.04  
L-index

#	Paper	IF	Citations
99	Superconducting high pressure phase of germane. <i>Physical Review Letters</i> , <b>2008</b> , 101, 107002	7.4	204
98	Structures and potential superconductivity in at high pressure: en route to "metallic hydrogen". <i>Physical Review Letters</i> , <b>2006</b> , 96, 017006	7.4	174
97	High-pressure crystal structures and superconductivity of Stannane (SnH <sub>4</sub> ). <i>Proceedings of the National Academy of Sciences of the United States of America</i> , <b>2010</b> , 107, 1317-20	11.5	153
96	Novel structures and superconductivity of silane under pressure. <i>Physical Review Letters</i> , <b>2009</b> , 102, 087005	7.4	137
95	Two-Dimensional PC with Direct Band Gap and Anisotropic Carrier Mobility. <i>Journal of the American Chemical Society</i> , <b>2019</b> , 141, 1599-1605	16.4	76
94	Exotic behavior and crystal structures of calcium under pressure. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , <b>2010</b> , 107, 7646-51	11.5	74
93	Gold as a 6p-Element in Dense Lithium Aurides. <i>Journal of the American Chemical Society</i> , <b>2016</b> , 138, 4046-52	16.4	70
92	Anharmonic effects in atomic hydrogen: Superconductivity and lattice dynamical stability. <i>Physical Review B</i> , <b>2016</b> , 93,	3.3	60
91	Crystal structure of SiH <sub>4</sub> at high pressure. <i>Physical Review B</i> , <b>2007</b> , 76,	3.3	60
90	Anomalous High-Temperature Superconductivity in YH. <i>Advanced Materials</i> , <b>2021</b> , 33, e2006832	24	60
89	First-principles simulations of lithium melting: stability of the bcc phase close to melting. <i>Physical Review Letters</i> , <b>2010</b> , 104, 185701	7.4	59
88	Metallic and superconducting gallane under high pressure. <i>Physical Review B</i> , <b>2011</b> , 84,	3.3	58
87	Anharmonic stabilization of the high-pressure simple cubic phase of calcium. <i>Physical Review Letters</i> , <b>2011</b> , 106, 165501	7.4	56
86	Exotic high pressure behavior of light alkali metals, lithium and sodium. <i>European Physical Journal B</i> , <b>2011</b> , 81, 1-14	1.2	56
85	Pressure induced metallization of Germane. <i>Journal of Physics and Chemistry of Solids</i> , <b>2006</b> , 67, 2095-2099	3.3	55
84	Potential high-T <sub>c</sub> superconductivity in CaYH <sub>12</sub> under pressure. <i>Physical Review B</i> , <b>2019</b> , 99,	3.3	53
83	Theoretical study of the ground-state structures and properties of niobium hydrides under pressure. <i>Physical Review B</i> , <b>2013</b> , 88,	3.3	52

82	Predicted Pressure-Induced Superconducting Transition in Electride Li <sub>6</sub> P. <i>Physical Review Letters</i> , <b>2019</b> , 122, 097002	7.4	51
81	Relativistic effects and fully spin-polarized Fermi surface at the Tl/Si(111) surface. <i>Physical Review B</i> , <b>2011</b> , 84,	3.3	49
80	Giant anharmonicity suppresses superconductivity in AlH <sub>3</sub> under pressure. <i>Physical Review B</i> , <b>2010</b> , 82,	3.3	44
79	Phonon Collapse and Second-Order Phase Transition in Thermoelectric SnSe. <i>Physical Review Letters</i> , <b>2019</b> , 122, 075901	7.4	42
78	Complexity and Fermi surface deformation in compressed lithium. <i>Physical Review B</i> , <b>2006</b> , 74,	3.3	39
77	Pairing, Bonding, and the role of nonlocality in a dense lithium monolayer. <i>Physical Review B</i> , <b>2000</b> , 62, 8494-8499	3.3	32
76	A model for the velocity-dependent screening. <i>Nuclear Instruments &amp; Methods in Physics Research B</i> , <b>1996</b> , 115, 58-61	1.2	30
75	Efficient computation of magnon dispersions within time-dependent density functional theory using maximally localized Wannier functions. <i>Physical Review B</i> , <b>2012</b> , 85,	3.3	28
74	Structural, Vibrational, and Electronic Study of As <sub>2</sub> Te <sub>3</sub> under Compression. <i>Journal of Physical Chemistry C</i> , <b>2016</b> , 120, 19340-19352	3.8	28
73	Pressure-Induced Stable LiSP for High-Performance Lithium-Ion Batteries. <i>Journal of Physical Chemistry C</i> , <b>2017</b> , 121, 21199-21205	3.8	27
72	Enhanced Friedel structure and proton pairing in dense solid hydrogen. <i>Physical Review Letters</i> , <b>2003</b> , 90, 035501	7.4	27
71	Fermi surface nesting and phonon instabilities in simple cubic calcium. <i>High Pressure Research</i> , <b>2008</b> , 28, 443-448	1.6	24
70	Tight-binding models for ultracold atoms in honeycomb optical lattices. <i>Physical Review A</i> , <b>2013</b> , 87,	2.6	22
69	Quadratic induced polarization by an external heavy charge in an electron gas. <i>Physical Review B</i> , <b>1997</b> , 56, 15654-15664	3.3	22
68	Nonmetallic FeH <sub>6</sub> under High Pressure. <i>Journal of Physical Chemistry C</i> , <b>2018</b> , 122, 12022-12028	3.8	21
67	Lindemann criterion and the anomalous melting curve of sodium. <i>Journal of Physics and Chemistry of Solids</i> , <b>2008</b> , 69, 2151-2154	3.9	21
66	Pressure induced complexity in a lithium monolayer: Ab initio calculations. <i>Physical Review B</i> , <b>2005</b> , 72,	3.3	21
65	Quadratic electronic response of a two-dimensional electron gas. <i>Physical Review B</i> , <b>1999</b> , 59, 10145-10151	3.3	21

64	Strong anharmonicity and high thermoelectric efficiency in high-temperature SnS from first principles. <i>Physical Review B</i> , <b>2019</b> , 100,	3.3	21
63	LiB and its boron-deficient variants under pressure. <i>Physical Review B</i> , <b>2012</b> , 86,	3.3	20
62	Spin-flip transitions induced by time-dependent electric fields in surfaces with strong spin-orbit interaction. <i>Physical Review Letters</i> , <b>2012</b> , 109, 156401	7.4	18
61	No evidence of metallic methane at high pressure. <i>High Pressure Research</i> , <b>2006</b> , 26, 369-375	1.6	18
60	Ferromagnetic instabilities in atomically thin lithium and sodium wires. <i>International Journal of Quantum Chemistry</i> , <b>2003</b> , 91, 239-244	2.1	18
59	A New Three-Dimensional Subsulfide IrInS with Dirac Semimetal Behavior. <i>Journal of the American Chemical Society</i> , <b>2019</b> , 141, 19130-19137	16.4	17
58	Anharmonic enhancement of superconductivity in metallic molecular Cmca - 4 hydrogen at high pressure: a first-principles study. <i>Journal of Physics Condensed Matter</i> , <b>2016</b> , 28, 494001	1.8	17
57	First-principles study of crystal structures and superconductivity of ternary YSH6 and LaSH6 at high pressures. <i>Physical Review B</i> , <b>2019</b> , 100,	3.3	16
56	Energy loss spectra of lithium under pressure. <i>New Journal of Physics</i> , <b>2008</b> , 10, 053035	2.9	16
55	Ab initio dynamical response of metal monolayers. <i>Physical Review B</i> , <b>2003</b> , 67,	3.3	16
54	Self-consistent tight-binding description of Dirac points moving and merging in two-dimensional optical lattices. <i>Physical Review A</i> , <b>2013</b> , 88,	2.6	15
53	Energy-loss rates of heavy and light charged particles in a two-dimensional electron gas. <i>Physical Review B</i> , <b>1997</b> , 55, 12864-12867	3.3	15
52	Strong variation of dielectric response and optical properties of lithium under pressure. <i>Physical Review B</i> , <b>2007</b> , 75,	3.3	15
51	Pressure induced phase transitions in TiH <sub>2</sub> . <i>Journal of Applied Physics</i> , <b>2013</b> , 113, 103512	2.5	14
50	Electronic collective excitations in compressed lithium from ab initio calculations: Importance and anisotropy of local-field effects at large momenta. <i>Physical Review B</i> , <b>2010</b> , 81,	3.3	14
49	Ab initio study of superconducting hexagonal Be <sub>2</sub> Li under pressure. <i>Physical Review B</i> , <b>2008</b> , 78,	3.3	13
48	Plasmon excitation by charged particles interacting with metal surfaces. <i>Physics Letters, Section A: General, Atomic and Solid State Physics</i> , <b>1999</b> , 256, 405-410	2.3	13
47	Prediction of high-T <sub>c</sub> superconductivity in ternary lanthanum borohydrides. <i>Physical Review B</i> , <b>2021</b> , 104,	3.3	13

46	Nonlinear effects on charged particle interactions in matter. <i>Nuclear Instruments &amp; Methods in Physics Research B</i> , <b>1995</b> , 99, 187-191	1.2	11
45	Strong Electron-Phonon and Band Structure Effects in the Optical Properties of High Pressure Metallic Hydrogen. <i>Physical Review Letters</i> , <b>2018</b> , 120, 057402	7.4	10
44	Spin-flip transitions and departure from the Rashba model in the Au(111) surface. <i>Physical Review B</i> , <b>2013</b> , 88,	3.3	10
43	Breakdown of the Peierls substitution for the Haldane model with ultracold atoms. <i>Physical Review A</i> , <b>2014</b> , 90,	2.6	9
42	Superconducting boron allotropes. <i>Physical Review B</i> , <b>2020</b> , 101,	3.3	8
41	Nonlinear wake in the random-phase-approximation. <i>Nuclear Instruments &amp; Methods in Physics Research B</i> , <b>1995</b> , 96, 604-609	1.2	8
40	Anisotropic and High-Mobility CS Monolayer as a Photocatalyst for Water Splitting. <i>Journal of Physical Chemistry Letters</i> , <b>2021</b> , 12, 8320-8327	6.4	8
39	Novel superhard boron-rich nitrides under pressure. <i>Science China Materials</i> , <b>2020</b> , 63, 2358-2364	7.1	7
38	Anisotropic PC6N Monolayer with Wide Band Gap and Ultrahigh Carrier Mobility. <i>Journal of Physical Chemistry C</i> , <b>2020</b> , 124, 4330-4337	3.8	7
37	Phase diagrams and electronic properties of B-S and H-B-S systems under high pressure. <i>Physical Review B</i> , <b>2019</b> , 100,	3.3	7
36	Hard and superconducting cubic boron phase via swarm-intelligence structural prediction driven by a machine-learning potential. <i>Physical Review B</i> , <b>2021</b> , 103,	3.3	7
35	Ab initio analysis of plasmon dispersion in sodium under pressure. <i>Physical Review B</i> , <b>2014</b> , 89,	3.3	6
34	Hydrodynamic approximation for the nonlinear response of a metal surface. <i>Physical Review B</i> , <b>1999</b> , 60, 16176-16185	3.3	6
33	Weyl fermions, Fermi arcs, and minority-spin carriers in ferromagnetic CoS. <i>Science Advances</i> , <b>2020</b> , 6,	14.3	6
32	Isotope effect in the superconducting high-pressure simple cubic phase of calcium from first principles. <i>Journal of Applied Physics</i> , <b>2012</b> , 111, 112604	2.5	5
31	Optical properties of calcium under pressure from first-principles calculations. <i>Physical Review B</i> , <b>2012</b> , 86,	3.3	5
30	Undamped low-energy plasmon in AlH <sub>3</sub> at high pressure. <i>Physical Review B</i> , <b>2010</b> , 82,	3.3	5
29	Nesting Induced Peierls-Type Instability for Compressed Li-cl <sub>16</sub> . <i>Journal of the Physical Society of Japan</i> , <b>2007</b> , 76, 21-22	1.5	5

28	Nonlinear quantum hydrodynamical model of the electron gas. <i>Nuclear Instruments &amp; Methods in Physics Research B</i> , <b>1996</b> , 115, 70-74	1.2	5
27	Structural and Superconducting Properties of Tungsten Hydrides Under High Pressure. <i>Frontiers in Physics</i> , <b>2018</b> , 6,	3.9	5
26	The Subchalcogenides IrInQ (Q = S, Se, Te): Dirac Semimetal Candidates with Re-entrant Structural Modulation. <i>Journal of the American Chemical Society</i> , <b>2020</b> , 142, 6312-6323	16.4	4
25	Prediction of superconductivity in pressure-induced new silicon boride phases. <i>Physical Review B</i> , <b>2020</b> , 101,	3.3	4
24	Anharmonicity in aluminum hydride at high pressures. <i>High Pressure Research</i> , <b>2011</b> , 31, 30-34	1.6	4
23	Enhanced Anharmonicity Under Pressure. <i>Journal of Physics: Conference Series</i> , <b>2012</b> , 377, 012060	0.3	4
22	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> , <b>2010</b> , 71, 1159-1164	3.9	4
21	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> , <b>1998</b> , 135, 97-102	1.2	4
20	Achieving high hydrogen evolution reaction activity of a MoC monolayer. <i>Physical Chemistry Chemical Physics</i> , <b>2020</b> , 22, 26189-26199	3.6	4
19	Ba with Unusual Oxidation States in Ba Chalcogenides under Pressure. <i>Journal of Physical Chemistry Letters</i> , <b>2021</b> , 12, 4203-4210	6.4	4
18	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> , <b>2020</b> , 3, 014001	4.2	4
17	Wide Band Gap PS Monolayer with Anisotropic and Ultrahigh Carrier Mobility. <i>Journal of Physical Chemistry Letters</i> , <b>2021</b> , 12, 8481-8488	6.4	4
16	High pressure phases of different tetraboranes. <i>High Pressure Research</i> , <b>2014</b> , 34, 59-69	1.6	3
15	Dynamical response function of a compressed lithium monolayer. <i>Surface Science</i> , <b>2006</b> , 600, 3856-3859	1.8	3
14	Anharmonicity and the isotope effect in superconducting lithium at high pressures: A first-principles approach. <i>Physical Review B</i> , <b>2017</b> , 96,	3.3	2
13	Ab initio analysis of the topological phase diagram of the Haldane model. <i>Physical Review B</i> , <b>2015</b> , 92,	3.3	2
12	Ab initio superconducting temperature of BaSi <sub>2</sub> at ambient pressure. <i>Journal of Physics: Conference Series</i> , <b>2010</b> , 215, 012109	0.3	2
11	Fermi surface deformation in lithium under high pressure. <i>High Pressure Research</i> , <b>2006</b> , 26, 461-465	1.6	2

10	On the validity of perturbative treatments for the static screening in a charged-boson gas. <i>Journal of Physics Condensed Matter</i> , <b>1999</b> , 11, 3943-3949	1.8	2
9	Superconducting LaP2H2 with graphenelike phosphorus layers. <i>Physical Review B</i> , <b>2022</b> , 105,	3.3	2
8	An epilepsy-causing mutation leads to co-translational misfolding of the Kv7.2 channel. <i>BMC Biology</i> , <b>2021</b> , 19, 109	7.3	2
7	Structural characterization of slightly boron-deficient LiB, LiB0.9 and LiB0.8, under pressure. <i>Journal of Physics Condensed Matter</i> , <b>2014</b> , 26, 475402	1.8	1
6	Anomalous static electronic screening in compressed lithium. <i>Journal of Physics: Conference Series</i> , <b>2008</b> , 121, 012007	0.3	1
5	Do calmodulin binding IQ motifs have built-in capping domains?. <i>Protein Science</i> , <b>2021</b> , 30, 2029-2041	6.3	1
4	Theoretical study of topological properties of ferromagnetic pyrite CoS2. <i>Journal Physics D: Applied Physics</i> , <b>2022</b> , 55, 304004	3	0
3	Plasmons in Li under compression. <i>Journal of Physics Condensed Matter</i> , <b>2019</b> , 31, 185501	1.8	
2	Quadratic Response Solutions for Different Nonlinear Approaches of Static Screening: A Comparative Study <b>2002</b> , 657-661		
1	Phase transitions of alkaline-earth metal sulfides under pressure. <i>Materials Research Express</i> , <b>2021</b> , 8, 065902	1.7	