

Murat Durandurdu

List of Publications by Year in descending order

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100
papers

1,205
citations

430754

18
h-index

434063

31
g-index

100
all docs

100
docs citations

100
times ranked

1334
citing authors

#	ARTICLE	IF	CITATIONS
1	Transformation pathways of silica under high pressure. Nature Materials, 2006, 5, 977-981.	13.3	91
2	Ab initio simulation of first-order amorphous-to-amorphous phase transition of silicon. Physical Review B, 2001, 64, .	1.1	80
3	Simulation of pressure-induced polyamorphism in a chalcogenide glass GeSe ₂ . Physical Review B, 2002, 65, .	1.1	78
4	First principles study of structural phase stability of wide-gap semiconductors MgTe, MgS and MgSe. Computational Materials Science, 2009, 47, 593-598.	1.4	71
5	First-order pressure-induced polyamorphism in germanium. Physical Review B, 2002, 66, .	1.1	41
6	High-pressure phases of amorphous and crystalline silicon. Physical Review B, 2003, 67, .	1.1	40
7	High-pressure phases of ZrO ₂ : An ab initio constant-pressure study. Physical Review B, 2009, 79, .	1.1	39
8	Ab initio simulations of the structural phase transformation of SiC at high pressure. Physical Review B, 2007, 75, .	1.1	36
9	Pressure-induced phase transition of SiC. Journal of Physics Condensed Matter, 2004, 16, 4411-4417.	0.7	35
10	Pressure-induced phase transition in wurtzite ZnS: An ab initio constant pressure study. Journal of Physics and Chemistry of Solids, 2009, 70, 645-649.	1.9	31
11	Ab initio modeling of metallic Pd ₈₀ Si ₂₀ glass. Computational Materials Science, 2012, 65, 44-47.	1.4	29
12	Ab initio simulation of high-pressure phases of GaAs. Physical Review B, 2002, 66, .	1.1	28
13	Approximate ab initio calculations of electronic structure of amorphous silicon. Physical Review B, 2000, 62, 15307-15310.	1.1	26
14	Formation of a Cmcm phase in SnS at high pressure; an ab initio constant pressure study. Solid State Communications, 2010, 150, 870-874.	0.9	24
15	Pressure-induced phase transition of zinc-blende AlN: An ab initio molecular dynamics study. Journal of Physics and Chemistry of Solids, 2008, 69, 2894-2897.	1.9	22
16	Pressure-induced phase transition in AlN: An ab initio molecular dynamics study. Journal of Alloys and Compounds, 2009, 480, 917-921.	2.8	22
17	New B ₂ O ₃ Crystals Predicted from Concurrent Molecular Dynamics Simulations and First-Principles Calculations. Journal of Physical Chemistry C, 2007, 111, 13712-13720.	1.5	21
18	High-density amorphous phase of GeS ₂ under pressure. Physical Review B, 2009, 79, .		

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19	Pressure-induced Amorphization of MOF: A First Principles Study. ChemistrySelect, 2018, 3, 8056-8063.	0.7	18
20	Cmcmphase of GeS at high pressure. Physical Review B, 2005, 72, .	1.1	17
21	Electronic and mechanical properties of wurtzite type SiC nanowires. Physica Status Solidi (B): Basic Research, 2006, 243, R37-R39.	0.7	17
22	Pressure-induced phase transition of BeO. Solid State Communications, 2009, 149, 345-348.	0.9	17
23	Structural phase transition of germanium under uniaxial stress: An ab initio study. Physical Review B, 2005, 71, .	1.1	16
24	Pressure-induced amorphization, mechanical and electronic properties of zeolitic imidazolate framework (ZIF-8). Materials Chemistry and Physics, 2020, 240, 122222.	2.0	16
25	Structural phase transition of gold under uniaxial, tensile, and triaxial stresses: An ab initio study. Physical Review B, 2007, 76, .	1.1	15
26	Ab initio molecular dynamics study of pressure-induced phase transition in ZnS. Journal of Physics Condensed Matter, 2006, 18, 9483-9491.	0.7	14
27	Ab initio modeling of small diameter silicon nanowires. Physica Status Solidi (B): Basic Research, 2006, 243, R7-R9.	0.7	14
28	Hexagonal nanosheets in amorphous BN: A first principles study. Journal of Non-Crystalline Solids, 2015, 427, 41-45.	1.5	13
29	Ab initio simulation of pressure-induced low-energy excitations in amorphous silicon. Physical Review B, 2002, 66, .	1.1	12
30	Pressure-induced phase transformation of BaS: An ab initio constant pressure study. Chemical Physics, 2010, 367, 80-82.	0.9	12
31	Diamond to β -Sn phase transition of silicon under hydrostatic and nonhydrostatic compressions. Journal of Physics Condensed Matter, 2008, 20, 325232.	0.7	11
32	The structural phase transition of ZnSe under hydrostatic and nonhydrostatic compressions: an ab initio molecular dynamics study. Journal of Physics Condensed Matter, 2009, 21, 125403.	0.7	11
33	Pressure-induced phase transformation of 4H-SiC: An ab initio constant-pressure study. Europhysics Letters, 2009, 87, 36001.	0.7	11
34	Novel high-pressure phase of ZrO ₂ : An ab initio prediction. Journal of Solid State Chemistry, 2015, 230, 233-236.	1.4	10
35	Liquid boron and amorphous boron: An ab initio molecular dynamics study. Journal of Non-Crystalline Solids, 2015, 417-418, 10-14.	1.5	10
36	Pressure-induced phase transformation in CdO: An ab initio constant-pressure study. Europhysics Letters, 2008, 84, 66003.	0.7	9

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37	Orthorhombic intermediate phases for the wurtzite-to-rocksalt phase transformation of CdSe: An ab initio constant pressure study. <i>Chemical Physics</i> , 2010, 369, 55-58.	0.9	9
38	Pressure-induced structural phase transition of paracrystalline silicon. <i>Physical Review B</i> , 2002, 66, .	1.1	8
39	Phase transformation of 6H-SiC at high pressure: An ab initio constant-pressure study. <i>Europhysics Letters</i> , 2008, 84, 26003.	0.7	8
40	New transformation mechanism for a zinc-blende to rocksalt phase transformation in MgS. <i>Journal of Physics Condensed Matter</i> , 2009, 21, 452204.	0.7	8
41	Polyamorphism in Aluminum Nitride: A First Principles Molecular Dynamics Study. <i>Journal of the American Ceramic Society</i> , 2016, 99, 1594-1600.	1.9	8
42	Ab initio simulation of the rhombohedral to simple-cubic transition in arsenic. <i>Physical Review B</i> , 2005, 72, .	1.1	7
43	Formation of an anatase-like phase in silica under anisotropic stress: An ab initio constant-pressure study. <i>Physical Review B</i> , 2009, 80, .	1.1	7
44	Expanded phase of ZrO ₂ : An ab initio constant-pressure study. <i>Europhysics Letters</i> , 2009, 88, 66001.	0.7	7
45	Atomic structure of amorphous CdO from first principles simulations. <i>Journal of Non-Crystalline Solids</i> , 2015, 412, 11-15.	1.5	7
46	Amorphous zirconia: <i>ab initio</i> molecular dynamics simulations. <i>Philosophical Magazine</i> , 2017, 97, 1334-1345.	0.7	7
47	Phase transition of GeSe ₂ at high pressure. <i>Physica Status Solidi (B): Basic Research</i> , 2005, 242, 3085-3090.	0.7	6
48	Formation of Cotunnite Phase in ZrO ₂ under Uniaxial Stress: A First Principles Study. <i>Journal of the American Ceramic Society</i> , 2011, 94, 932-937.	1.9	6
49	Two successive amorphous to amorphous phase transformations in TiO ₂ . <i>Journal of the American Ceramic Society</i> , 2017, 100, 3903-3911.	1.9	6
50	Hard boron rich boron nitride nanoglasses. <i>Journal of the American Ceramic Society</i> , 2018, 101, 1929-1939.	1.9	6
51	Amorphous boron carbide from ab initio simulations. <i>Computational Materials Science</i> , 2020, 173, 109397.	1.4	6
52	Pressure-induced amorphous-to-amorphous phase transition in GaAs. <i>Physical Review B</i> , 2004, 70, .	1.1	5
53	Transition pathway in GaAs under uniaxial stress: an ab initio study. <i>Journal of Physics Condensed Matter</i> , 2006, 18, 4887-4894.	0.7	5
54	Ab initio simulation of polyamorphic phase transition in hydrogenated silicon. <i>Physical Review B</i> , 2006, 73, .	1.1	5

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55	Vibrational properties of amorphous germanium under pressure and its thermal expansion and Grüneisen parameters. Journal of Non-Crystalline Solids, 2010, 356, 977-981.	1.5	5
56	Uncovering Nanoclusters in Amorphous AlN: An <i>Ab Initio</i> Study. Journal of the American Ceramic Society, 2015, 98, 1095-1098.	1.9	5
57	Amorphous boron nitride at high pressure. Philosophical Magazine, 2016, 96, 1950-1964.	0.7	5
58	Hydrogenated amorphous boron nitride: A first principles study. Journal of Non-Crystalline Solids, 2018, 502, 159-163.	1.5	5
59	Amorphous silicon hexaboride at high pressure. Philosophical Magazine, 2020, 100, 1818-1833.	0.7	5
60	An ab initio constant-pressure study of pressure-induced phase transition of MgSe. Europhysics Letters, 2008, 84, 56001.	0.7	4
61	Ab initio molecular dynamics study of pressure-induced phase transformation in KCl. Computational Materials Science, 2010, 48, 672-676.	1.4	4
62	Nanosize icosahedral quasicrystal in Mg ₉₀ Ca ₁₀ glass: An ab initio molecular dynamics study. Journal of Chemical Physics, 2012, 137, 034503.	1.2	4
63	Nanosegregated amorphous AlB ₂ alloy. Philosophical Magazine, 2016, 96, 3200-3210.	0.7	4
64	Permanent densification of amorphous zinc oxide under pressure: A first principles study. Journal of Non-Crystalline Solids, 2018, 481, 27-32.	1.5	4
65	Amorphous boron suboxide. Journal of the American Ceramic Society, 2019, 102, 4546-4554.	1.9	4
66	Very low density amorphous phase of zircon. Journal of Non-Crystalline Solids, 2019, 513, 137-143.	1.5	4
67	Fcc-to-bct phase transformation of aluminum under triaxial stresses: an ab initio constant pressure study. European Physical Journal B, 2009, 72, 241-245.	0.6	3
68	Formation of a two-dimensional layered structure in silica under shear stresses: An <i>ab initio</i> study. Physical Review B, 2010, 81, .	1.1	3
69	Atomic structure of amorphous Mg ₄₀ Cu ₃₅ Ti ₂₅ alloy: An ab initio molecular dynamics study. Solid State Communications, 2013, 154, 30-33.	0.9	3
70	New high-pressure phase of MgH ₂ : An ab initio constant-pressure study. Europhysics Letters, 2014, 105, 46001.	0.7	3
71	Local structure of As ₂ O ₃ glass from first principles simulations. Journal of Non-Crystalline Solids, 2016, 436, 18-21.	1.5	3
72	Densification of amorphous boron under pressure. Journal of Non-Crystalline Solids, 2017, 471, 274-279.	1.5	3

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73	Amorphous silicon hexaboride: a first-principles study. Philosophical Magazine, 2018, 98, 2723-2733.	0.7	3
74	An in-depth investigation of Mg-Zn-Ca metallic glasses: A first principles study. Computational Materials Science, 2018, 153, 326-337.	1.4	3
75	Phase transition of ZrN under pressure. Philosophical Magazine, 2019, 99, 942-955.	0.7	3
76	Tetrahedral amorphous boron nitride: A hard material. Journal of the American Ceramic Society, 2020, 103, 973-978.	1.9	3
77	Theoretical investigation of substituent effects on the relative stabilities and electronic structure of [BnXn]2 ⁺ clusters. Journal of Molecular Modeling, 2021, 27, 365.	0.8	3
78	Nanoscale icosahedral packing in amorphous Mg 50 Ni 50 : An ab initio study. Europhysics Letters, 2012, 100, 26002.	0.7	2
79	High-pressure phase transitions of TiN: an ab initio constant pressure study. Philosophical Magazine, 2015, 95, 2376-2384.	0.7	2
80	High pressure modifications in amorphous boron suboxide: An ab initio study. Ceramics International, 2020, 46, 5968-5975.	2.3	2
81	Ab initio simulation of amorphous BC3. Computational Materials Science, 2020, 178, 109622.	1.4	2
82	A first principles study of amorphous and crystalline silicon tetraboride. Materials Chemistry and Physics, 2021, 258, 123928.	2.0	2
83	Amorphous boron phosphide: An ab initio investigation. Journal of Non-Crystalline Solids, 2021, 570, 121006.	1.5	2
84	Mechanically Controlled, Seeded Formation of a Nanoscale Metastable Phase in Ionic Compounds. Nano Letters, 2004, 4, 1769-1773.	4.5	1
85	Ferromagnetism in amorphous MgO. Philosophical Magazine, 2017, 97, 2129-2141.	0.7	1
86	MgCu metallic glass. Philosophical Magazine, 2018, 98, 633-645.	0.7	1
87	Solute aggregation in Ca72Zn28 metallic glass. Journal of Non-Crystalline Solids, 2018, 500, 410-416.	1.5	1
88	Amorphous zirconia at high pressure. Journal of the American Ceramic Society, 2018, 101, 5411-5418.	1.9	1
89	Amorphous boron arsenide. Journal of Non-Crystalline Solids, 2019, 524, 119656.	1.5	1
90	Liquid and amorphous states of boron subarsenide. Journal of the American Ceramic Society, 2020, 103, 176-182.	1.9	1

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91	Stoichiometric amorphous boron carbide (BC). Journal of Materials Science, 2020, 55, 14709-14716.	1.7	1
92	Amorphous silicon triboride: A first principles study. Journal of Non-Crystalline Solids, 2020, 536, 119995.	1.5	1
93	Formation of a very high-density amorphous phase of carbon and its crystallization into a simple cubic structure at high pressure. Computational Materials Science, 2021, 200, 110822.	1.4	1
94	Amorphous BC ₅ from first principles calculations. Journal of Non-Crystalline Solids, 2022, 592, 121743.	1.5	1
95	Formation of Anatase Phase in HfO ₂ in Tensile Stress: An <i>Ab Initio</i> Study. Journal of the American Ceramic Society, 2010, 93, 1467-1469.	1.9	0
96	n-type conductivity in Si-doped amorphous AlN: an <i>ab initio</i> investigation. Philosophical Magazine, 2016, 96, 1110-1121.	0.7	0
97	Pressure-induced phase transformations in amorphous arsenic. Journal of Non-Crystalline Solids, 2016, 437, 6-9.	1.5	0
98	High-density amorphous phase of CdO. Journal of Non-Crystalline Solids, 2017, 463, 64-67.	1.5	0
99	Amorphous magnesium silicide. Journal of Non-Crystalline Solids, 2018, 498, 118-124.	1.5	0
100	Amorphous zircon at high pressure. Journal of Physics and Chemistry of Solids, 2021, 153, 109991.	1.9	0