Tahir Cagin

List of Publications by Year
in descending order

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112	9,594	41258	35952
papers	citations	49 h-index	97 g-index

114	114	114	10005
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Thermal conductivity of carbon nanotubes. Nanotechnology, 2000, 11, 65-69.	1.3	988
2	Structure of PAMAM Dendrimers:Â Generations 1 through 11. Macromolecules, 2004, 37, 6236-6254.	2.2	455
3	Thermal conductivity of BN-C nanostructures. Physical Review B, 2012, 86, .	1.1	429
4	Nanophase-Segregation and Transport in Nafion 117 from Molecular Dynamics Simulations:Â Effect of Monomeric Sequence. Journal of Physical Chemistry B, 2004, 108, 3149-3157.	1.2	425
5	Effect of Solvent and pH on the Structure of PAMAM Dendrimers. Macromolecules, 2005, 38, 979-991.	2.2	389
6	Melting and crystallization in Ni nanoclusters: The mesoscale regime. Journal of Chemical Physics, 2001, 115, 385-394.	1.2	345
7	Construction of hierarchically porous metalâ€“organic frameworks through linker labilization. Nature Communications, 2017, 8, 15356.	5.8	326
8	Control of Thermal and Electronic Transport in Defect-Engineered Graphene Nanoribbons. ACS Nano, 2011, 5, 3779-3787.	7.3	320
9	Thermal conductivity of diamond and related materials from molecular dynamics simulations. Journal of Chemical Physics, 2000, 113, 6888-6900.	1.2	307
10	Strain Rate Induced Amorphization in Metallic Nanowires. Physical Review Letters, 1999, 82, 2900-2903.	2.9	268
11	Characterization of thermal transport in low-dimensional boron nitride nanostructures. Physical Review B, 2011, 84, .	1.1	264
12	Molecular-dynamics simulations of glass formation and crystallization in binary liquid metals:â€ƒCu-Ag and Cu-Ni. Physical Review B, 1999, 59, 3527-3533.	1.1	252
13	Maximum superheating and undercooling: Systematics, molecular dynamics simulations, and dynamic experiments. Physical Review B, 2003, 68, .	1.1	234
14	Molecular dynamics study of the binaryCu46Zr54metallic glass motivated by experiments: Glass formation and atomic-level structure. Physical Review B, 2005, 71, .	1.1	227
15	Adhesion and nonwetting-wetting transition in theAl/Î±â^'Al2O3interface. Physical Review B, 2004, 69, .	1.1	184
16	Morse Stretch Potential Charge Equilibrium Force Field for Ceramics: Application to the Quartz-Stishovite Phase Transition and to Silica Glass. Physical Review Letters, 1999, 82, 1708-1711.	2.9	173
17	Retrosynthesis of multi-component metalâ^'organic frameworks. Nature Communications, 2018, 9, 808.	5.8	159
18	Molecular dynamics simulations of thermal resistance at the liquid-solid interface. Journal of Chemical Physics, 2008, 129, 174701.	1.2	146

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19	Factors affecting molecular dynamics simulated vitreous silica structures. Journal of Non-Crystalline Solids, 1999, 253, 133-142.	1.5	121
20	The ferroelectric and cubic phases in BaTiO3 ferroelectrics are also antiferroelectric. Proceedings of the National Academy of Sciences of the United States of America, 2006, 103, 14695-14700.	3.3	119
21	Calculation of Mechanical, Thermodynamic and Transport Properties of Metallic Glass Formers. Materials Research Society Symposia Proceedings, 1998, 554, 43.	0.1	117
22	Position of K Atoms in Doped Single-Walled Carbon Nanotube Crystals. Physical Review Letters, 1998, 80, 5556-5559.	2.9	117
23	A bottom-up route to enhance thermoelectric figures of merit in graphene nanoribbons. Scientific Reports, 2013, 3, 1228.	1.6	117
24	Molecular Modeling of Polycarbonate. 1. Force Field, Static Structure, and Mechanical Properties. Macromolecules, 1994, 27, 2383-2391.	2.2	111
25	Wetting of crystalline polymer surfaces: A molecular dynamics simulation. Journal of Chemical Physics, 1995, 103, 9053-9061.	1.2	109
26	Thermal transport properties of MoS₂and MoSe₂monolayers. Nanotechnology, 2016, 27, 055703.	1.3	108
27	Molecular dynamics with a variable number of molecules. Molecular Physics, 1991, 72, 169-175.	0.8	100
28	Phonon Engineering in Carbon Nanotubes by Controlling Defect Concentration. Nano Letters, 2011, 11, 4971-4977.	4.5	99
29	Dynamics of Bengal Rose Encapsulated in the Meijer Dendrimer Box. Journal of the American Chemical Society, 1997, 119, 7458-7462.	6.6	93
30	Critical behavior in spallation failure of metals. Physical Review B, 2001, 63, .	1.1	92
31	Thermal interactions in nanoscale fluid flow: molecular dynamics simulations with solidâ€“liquid interfaces. Microfluidics and Nanofluidics, 2008, 5, 551-559.	1.0	92
32	Grand Molecular Dynamics: A Method for Open Systems. Molecular Simulation, 1991, 6, 5-26.	0.9	86
33	Dynamic response of<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow><mml:mtext>Cu</mml:mtext></mml:mrow><mml:mrow><mml:mn>46</mml:mn> glass to high-strain-rate shock loading: Plasticity, spall, and atomic-level structures. Physical Review B, 2010, 81, .	1.1	85
34	Criteria for formation of metallic glasses: The role of atomic size ratio. Journal of Chemical Physics, 2003, 119, 9858-9870.	1.2	81
35	Viscosities of liquid metal alloys from nonequilibrium molecular dynamics. Journal of Computer-Aided Materials Design, 2001, 8, 233-243.	0.7	79
36	Phase diagram of MgO from density-functional theory and molecular-dynamics simulations. Physical Review B, 1999, 60, 15084-15093.	1.1	77

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37	Sugar, water and free volume networks in concentrated sucrose solutions. Chemical Physics Letters, 2003, 377, 469-474.	1.2	72
38	Dynamic simulations of water at constant chemical potential. Journal of Chemical Physics, 1992, 96, 1333-1342.	1.2	65
39	Continuous Variation of Lattice Dimensions and Pore Sizes in Metalâ€“Organic Frameworks. Journal of the American Chemical Society, 2020, 142, 4732-4738.	6.6	65
40	Nanophase Segregation and Water Dynamics in the Dendrion Diblock Copolymer Formed from the FrÃ©chet Polyaryl Ethereal Dendrimer and Linear PTFE. Journal of Physical Chemistry B, 2005, 109, 10154-10167.	1.2	62
41	Fundamental treatment of molecular-dynamics ensembles. Physical Review A, 1988, 37, 247-251.	1.0	58
42	Simulation and experiments on friction and wear of diamond: a material for MEMS and NEMS application. Nanotechnology, 1999, 10, 278-284.	1.3	58
43	Report from the third workshop on future directions of solid-state chemistry: The status of solid-state chemistry and its impact in the physical sciences. Progress in Solid State Chemistry, 2008, 36, 1-133.	3.9	58
44	Viscous heating in nanoscale shear driven liquid flows. Microfluidics and Nanofluidics, 2010, 9, 31-40.	1.0	58
45	Molecular modelling of dendrimers for nanoscale applications. Nanotechnology, 2000, 11, 77-84.	1.3	57
46	Friction anisotropy at Ni(100)/(100) interfaces:â€ƒMolecular dynamics studies. Physical Review B, 2002, 66, .	1.1	55
47	Local chain dynamics of a model polycarbonate near glass transition temperature: A molecular dynamics simulation. Macromolecular Theory and Simulations, 1997, 6, 83-102.	0.6	54
48	Influence of disorder on thermal transport properties of boron nitride nanostructures. Physical Review B, 2012, 86, .	1.1	54
49	Generalized extended empirical bond-order dependent force fields including nonbond interactions. Theoretical Chemistry Accounts, 1999, 102, 346-354.	0.5	53
50	Strong configurational dependence of elastic properties for a binary model metallic glass. Applied Physics Letters, 2006, 89, 151901.	1.5	53
51	Structure of polyamidoamide dendrimers up to limiting generations: A mesoscale description. Journal of Chemical Physics, 2009, 130, 144902.	1.2	46
52	The SAM Model for Wear Inhibitor Performance of Dithiophosphates on Iron Oxide. Journal of Physical Chemistry B, 1997, 101, 7702-7709.	1.2	44
53	Effect of cyclic chain architecture on properties of dilute solutions of polyethylene from molecular dynamics simulations. Journal of Chemical Physics, 2003, 119, 1843-1854.	1.2	44
54	Atomic simulations of kinetic friction and its velocity dependence atAlâˆ•AlandÎ±â€²Al2O3âˆ•Î±â€²Al2O3interfaces. Physical Review B, 2005, 72, .	1.1	42

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55	Multiscale modeling and simulation methods with applications to dendritic polymers. Computational and Theoretical Polymer Science, 2001, 11, 345-356.	1.1	41
56	High-Pressure Methane, Carbon Dioxide, and Nitrogen Adsorption on Amine-Impregnated Porous Montmorillonite Nanoclays. Journal of Chemical & Engineering Data, 2016, 61, 2749-2760.	1.0	38
57	Finite-temperature elasticity of fcc Al: Atomistic simulations and ultrasonic measurements. Physical Review B, 2011, 84, .	1.1	37
58	Strategies for multiscale modeling and simulation of organic materials: polymers and biopolymers. Computational and Theoretical Polymer Science, 2001, 11, 329-343.	1.1	36
59	Fluorescence Enhancement in the Solid State by Isolating Perylene Fluorophores in Metalâ€“Organic Frameworks. ACS Applied Materials & Interfaces, 2020, 12, 26727-26732.	4.0	36
60	Studies of fullerenes and carbon nanotubes by an extended bond order potential. Nanotechnology, 1999, 10, 263-268.	1.3	35
61	A multiscale approach for modeling crystalline solids. Journal of Computer-Aided Materials Design, 2001, 8, 127-149.	0.7	31
62	Molecular dynamics simulations to compute the bulk response of amorphous PMMA. Journal of Computer-Aided Materials Design, 2001, 8, 87-106.	0.7	31
63	Atomistic simulations of kinks in1/2aã€ˆ111ã€‰screw dislocations in bcc tantalum. Physical Review B, 2003, 68, .	1.1	30
64	Mechanisms of Nonexponential Relaxation in Supercooled Glucose Solutions:â€‰ the Role of Water Facilitation. Journal of Physical Chemistry A, 2004, 108, 3699-3712.	1.1	30
65	Origin of static friction and its relationship to adhesion at the atomic scale. Physical Review B, 2007, 75, .	1.1	30
66	A method for modeling icosahedral virions: Rotational symmetry boundary conditions. Journal of Computational Chemistry, 1991, 12, 627-634.	1.5	29
67	Investigation of effective mass of carriers in Bi2Te3/Sb2Te3 superlattices via electronic structure studies on its component crystals. Applied Physics Letters, 2006, 89, 152101.	1.5	29
68	Fast Ewald sums for general van der Waals potentials. Journal of Computational Chemistry, 1997, 18, 1365-1370.	1.5	26
69	Assessment of phenomenological models for viscosity of liquids based on nonequilibrium atomistic simulations of copper. Journal of Chemical Physics, 2005, 123, 104506.	1.2	26
70	Application of the Self-Assembled Monolayer (SAM) Model to Dithiophosphate and Dithiocarbamate Engine Wear Inhibitors. Journal of Physical Chemistry A, 2000, 104, 2508-2524.	1.1	25
71	Coarse grain modeling of polyimide copolymers. Polymer, 2010, 51, 2786-2794.	1.8	25
72	Isothermal molecular-dynamics ensembles. Physical Review A, 1988, 37, 4510-4513.	1.0	23

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73	Computational Materials Chemistry at the Nanoscale. Journal of Nanoparticle Research, 1999, 1, 51-69.	0.8	23
74	The MS-Q Force Field for Clay Minerals:Â Application to Oil Production. Journal of Physical Chemistry B, 2001, 105, 4122-4127.	1.2	23
75	Molecular dynamics modeling of stishovite. Earth and Planetary Science Letters, 2002, 202, 147-157.	1.8	21
76	Analysis of strain fields in silicon nanocrystals. Applied Physics Letters, 2009, 94, 191914.	1.5	21
77	Ab-initio studies of pressure induced phase transitions in BaO. Journal of Computer-Aided Materials Design, 2001, 8, 193-202.	0.7	19
78	Dynamic Charge Equilibration-Morse stretch force field: Application to energetics of pure silica zeolites. Journal of Computational Chemistry, 2002, 23, 1507-1514.	1.5	19
79	Simulation Studies on Hydrogen Sorption and Its Thermodynamics in Covalently Linked Carbon Nanotube Scaffold. Journal of Physical Chemistry B, 2010, 114, 13752-13763.	1.2	18
80	Thermal conductivity engineering of bulk and one-dimensional Si-Ge nanoarchitectures. Science and Technology of Advanced Materials, 2017, 18, 187-196.	2.8	18
81	Metalâ€“Organicâ€“Inorganic Nanocomposite Thermal Interface Materials with Ultralow Thermal Resistances. ACS Applied Materials & Interfaces, 2017, 9, 10120-10127.	4.0	17
82	The ReaxFF Polarizable Reactive Force Fields for Molecular Dynamics Simulation of Ferroelectrics. AIP Conference Proceedings, 2002, , .	0.3	16
83	Ab Initio Studies On Phase Behavior of Barium Titanate. Materials Research Society Symposia Proceedings, 2002, 718, 1.	0.1	14
84	Insights from theoretical calculations on structure, dynamics, phase behavior and hydrogen sorption in nanoporous metal organic frameworks. Computational and Theoretical Chemistry, 2012, 987, 42-56.	1.1	14
85	Thermodynamic Stability of Zimmerman Self-Assembled Dendritic Supramolecules from Atomistic Molecular Dynamics Simulations. Journal of Physical Chemistry B, 2004, 108, 10041-10052.	1.2	12
86	Electrophoretic Transport of Na⁺ and K⁺ Ions Within Cyclic Peptide Nanotubes. Journal of Physical Chemistry B, 2016, 120, 7872-7879.	1.2	12
87	Thermodynamic and Elastic Properties of Polyethylene at Elevated Temperatures. Materials Research Society Symposia Proceedings, 1992, 278, 61.	0.1	11
88	Theoretical studies on VPI-5. 3.. Computational Materials Science, 1999, 14, 135-137.	1.4	11
89	Equilibrium limit of thermal conduction and boundary scattering in nanostructures. Journal of Chemical Physics, 2014, 140, 244112.	1.2	11
90	Novel algorithms for massively parallel, long-term, simulation of molecular dynamics systems. Advances in Engineering Software, 1998, 29, 441-450.	1.8	10

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91	Thermo-mechanical stability and strength of peptide nanostructures from molecular dynamics: self-assembled cyclic peptide nanotubes. Nanotechnology, 2010, 21, 115703.	1.3	10
92	Shock compression and spallation of palladium bicrystals with a Î£5 grain boundary. Journal of Applied Physics, 2011, 109, .	1.1	10
93	Kinks in the a/2ã€ˆ111ã€‰ screw dislocation in Ta. Journal of Computer-Aided Materials Design, 2001, 8, 117-125.	0.7	7
94	Crack propagation in a Tantalum nano-slab. Journal of Computer-Aided Materials Design, 2001, 8, 151-159.	0.7	6
95	Molecular Dynamics Simulations of Glass Formation and Crystallization in Binary Liquid Metals. Journal of Metastable and Nanocrystalline Materials, 2003, 15-16, 181-186.	0.1	5
96	Pressure Induced Phase Transformations in Silica. Materials Research Society Symposia Proceedings, 1997, 492, 287.	0.1	4
97	Recent Advances in Simulation of Dendritic Polymers. Materials Research Society Symposia Proceedings, 1998, 543, 299.	0.1	2
98	Molecular Dynamics Simulations of Supercooled Liquid Metals and Glasses. Materials Research Society Symposia Proceedings, 2000, 644, 231.	0.1	2
99	MPiSIM: Massively parallel simulation tool for metallic system. Journal of Computer-Aided Materials Design, 2001, 8, 185-192.	0.7	2
100	Molecular-Level Modeling and Simulation in Process Safety. , 2016, , 111-210.		2
101	Deformation Behavior of FCC Crystalline Metallic Nanowires Under High Strain Rates. Materials Research Society Symposia Proceedings, 1998, 554, 367.	0.1	1
102	First principles multiscale modeling of physico-chemical aspects of tribology. Tribology Series, 2001, , 15-33.	0.1	1
103	Molecular Dynamics Simulations of Piezoelectric Materials for Energy Harvesting Applications. Materials Science Forum, 0, 792, 54-64.	0.3	1
104	Acetonitrile confined in carbon nanotubes, part I: Structure, dynamic and transport properties. Journal of Molecular Liquids, 2020, 311, 113053.	2.3	1
105	Diamond and Polycrystalline Diamond for MEMS Applications: Simulations and Experiments. Materials Research Society Symposia Proceedings, 1998, 546, 109.	0.1	0
106	Structural and Dynamic Properties of Hexadecane Lubricants under Shear Flow in a Confined Geometry. ACS Symposium Series, 2001, , 158-177.	0.5	0
107	Atomistic Simulation of kinks for 1/2a<111> Screw Dislocation in Ta. Materials Research Society Symposia Proceedings, 2001, 677, 7301.	0.1	0
108	Application of lightweight threading techniques to computational chemistry. Journal of Computer-Aided Materials Design, 2001, 8, 173-184.	0.7	0

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109	Finite-temperature Anisotropic Elastic Properties of Ni-Mn-In Magnetic Shape Memory Alloy. Materials Research Society Symposia Proceedings, 2009, 1200, 63.	0.1	0
110	Cluster-ion bombardment studies to reveal the amorphization mode in strained Si0.8Ge0.2. Philosophical Magazine Letters, 2012, 92, 625-632.	0.5	0
111	Influence of Core-Shell Architecture Parameters on Thermal Conductivity of Si-Ge Nanowires. Materials Research Society Symposia Proceedings, 2015, 1735, 68.	0.1	0
112	Tailoring Thermal Conductivity of Ge/Si Core-Shell Nanowires. , 2015, , 433-440.		0