Davide Donadio

List of Publications by Citations

142 papers	15,769 citations	45 h-index	125 g-index
154 ext. papers	18,899 ext. citations	6.5 avg, IF	7.04 L-index

#	Paper	IF	Citations
142	Canonical sampling through velocity rescaling. *Journal of Chemical Physics*, **2007**, 126, 014101	3.9	8131
141	PLUMED: A portable plugin for free-energy calculations with molecular dynamics. *Computer Physics Communications*, **2009**, 180, 1961-1972	4.2	1087
140	Length-dependent thermal conductivity in suspended single-layer graphene. *Nature Communications*, **2014**, 5, 3689	17.4	603
139	Promoting transparency and reproducibility in enhanced molecular simulations. *Nature Methods*, **2019**, 16, 670-673	21.6	271
138	Atomistic simulations of heat transport in silicon nanowires. *Physical Review Letters*, **2009**, 102, 195901	7.4	226
137	Freezing of a Lennard-Jones fluid: from nucleation to spinodal regime. *Physical Review Letters*, **2006**, 97, 105701	7.4	207
136	Homogeneous ice nucleation from supercooled water. *Physical Chemistry Chemical Physics*, **2011**, 13, 19807-13	3.6	199
135	Crystal structure transformations in SiO2 from classical and ab initio metadynamics. *Nature Materials*, **2006**, 5, 623-6	27	183
134	Metadynamics simulations of the high-pressure phases of silicon employing a high-dimensional neural network potential. *Physical Review Letters*, **2008**, 100, 185501	7.4	181
133	Thermal conductivity of isolated and interacting carbon nanotubes: comparing results from molecular dynamics and the boltzmann transport equation. *Physical Review Letters*, **2007**, 99, 255502	7.4	153
132	Force and heat current formulas for many-body potentials in molecular dynamics simulations with applications to thermal conductivity calculations. *Physical Review B*, **2015**, 92,	3.3	144
131	Temperature dependence of the thermal conductivity of thin silicon nanowires. *Nano Letters*, **2010**, 10, 847-51	11.5	134
130	Hamiltonian adaptive resolution simulation for molecular liquids. *Physical Review Letters*, **2013**, 110, 108301	7.4	127
129	First Principles Simulations of the Infrared Spectrum of Liquid Water Using Hybrid Density Functionals. *Journal of Chemical Theory and Computation*, **2011**, 7, 1443-9	6.4	127
128	Nanophononics: state of the art and perspectives. *European Physical Journal B*, **2016**, 89, 1	1.2	124
127	Divergence of the thermal conductivity in uniaxially strained graphene. *Physical Review B*, **2013**, 87,	3.3	116
126	Blocking Phonon Transport by Structural Resonances in Alloy-Based Nanophononic Metamaterials Leads to Ultralow Thermal Conductivity. *Physical Review Letters*, **2016**, 117, 025503	7.4	114

125	Thermal transport in nanoporous silicon: interplay between disorder at mesoscopic and atomic scales. *ACS Nano*, **2011**, 5, 1839-44	16.7	105
124	Experimental and theoretical evidence for bilayer-by-bilayer surface melting of crystalline ice. *Proceedings of the National Academy of Sciences of the United States of America*, **2017**, 114, 227-232	11.5	102
123	Hyperbranched unsaturated polyphosphates as a protective matrix for long-term photon upconversion in air. *Journal of the American Chemical Society*, **2014**, 136, 11057-64	16.4	101
122	Ice nucleation at the nanoscale probes no man's land of water. *Nature Communications*, **2013**, 4, 1887	17.4	101
121	Lattice thermal conductivity of semiconducting bulk materials: atomistic simulations. *Physical Chemistry Chemical Physics*, **2012**, 14, 16209-22	3.6	94
120	Highly anisotropic thermal conductivity of arsenene: An ab initio study. *Physical Review B*, **2016**, 93,	3.3	93
119	Heat transport in amorphous silicon: Interplay between morphology and disorder. *Applied Physics Letters*, **2011**, 98, 144101	3.4	93
118	Polyamorphism of ice at low temperatures from constant-pressure simulations. *Physical Review Letters*, **2004**, 92, 225702	7.4	91
117	Tuning thermal transport in ultrathin silicon membranes by surface nanoscale engineering. *ACS Nano*, **2015**, 9, 3820-8	16.7	86
116	Dehydroxylation and Silanization of the Surfaces of β-Cristobalite Silica: An ab Initio Simulation. *Journal of Physical Chemistry B*, **2001**, 105, 8007-8013	3.4	85
115	Growth of Nanostructured Carbon Films by Cluster Assembly. *Physical Review Letters*, **1999**, 83, 776-779	7.4	80
114	Thermal conductivity decomposition in two-dimensional materials: Application to graphene. *Physical Review B*, **2017**, 95,	3.3	78
113	Surface-induced crystallization in supercooled tetrahedral liquids. *Nature Materials*, **2009**, 8, 726-30	27	76
112	Evolution of the structure of amorphous ice: from low-density amorphous through high-density amorphous to very high-density amorphous ice. *Journal of Chemical Physics*, **2005**, 122, 134501	3.9	76
111	Stability of hydrocarbons at deep Earth pressures and temperatures. *Proceedings of the National Academy of Sciences of the United States of America*, **2011**, 108, 6843-6846	11.5	64
110	Monte carlo adaptive resolution simulation of multicomponent molecular liquids. *Physical Review Letters*, **2013**, 111, 060601	7.4	63
109	An electrochemical thermal transistor. *Nature Communications*, **2018**, 9, 4510	17.4	63
108	Topological defects and bulk melting of hexagonal ice. *Journal of Physical Chemistry B*, **2005**, 109, 5421-4	3.4	61

107	Particle formation in the emulsion-solvent evaporation process. *Small*, **2013**, 9, 3514-22	11	60
106	Microscopic Mechanism and Kinetics of Ice Formation at Complex Interfaces: Zooming in on Kaolinite. *Journal of Physical Chemistry Letters*, **2016**, 7, 2350-5	6.4	59
105	Pressure-induced phase transitions in silicon studied by neural network-based metadynamics simulations. *Physica Status Solidi (B): Basic Research*, **2008**, 245, 2618-2629	1.3	59
104	Ab initio simulations of photoinduced interconversions of oxygen deficient centers in amorphous silica. *Physical Review Letters*, **2001**, 87, 195504	7.4	59
103	Site Binding of Ca2+Ions to Polyacrylates in Water: A Molecular Dynamics Study of Coiling and Aggregation. *Macromolecules*, **2007**, 40, 3437-3442	5.5	58
102	Thermal transport in phase-change materials from atomistic simulations. *Physical Review B*, **2012**, 86,	3.3	57
101	Influence of thermostatting on nonequilibrium molecular dynamics simulations of heat conduction in solids. *Journal of Chemical Physics*, **2019**, 151, 234105	3.9	56
100	Molecular dynamics study of the solvation of calcium carbonate in water. *Journal of Physical Chemistry B*, **2007**, 111, 12219-27	3.4	55
99	Morphology and temperature dependence of the thermal conductivity of nanoporous SiGe. *Nano Letters*, **2011**, 11, 3608-11	11.5	49
98	Autocatalytic and cooperatively stabilized dissociation of water on a stepped platinum surface. *Journal of the American Chemical Society*, **2012**, 134, 19217-22	16.4	46
97	Statistical mechanics of Hamiltonian adaptive resolution simulations. *Journal of Chemical Physics*, **2015**, 142, 064115	3.9	45
96	Mechanical Tuning of Thermal Transport in a Molecular Junction. *Journal of Physical Chemistry C*, **2015**, 119, 24636-24642	3.8	44
95	Dimensionality and heat transport in Si-Ge superlattices. *Applied Physics Letters*, **2013**, 102, 073113	3.4	41
94	First-Principle Analysis of the IR Stretching Band of Liquid Water. *Journal of Physical Chemistry Letters*, **2010**, 1, 1398-1402	6.4	40
93	Modeling heat transport in crystals and glasses from a unified lattice-dynamical approach. *Nature Communications*, **2019**, 10, 3853	17.4	39
92	Nuclear Quantum Effects in Water: A Multiscale Study. *Journal of Chemical Theory and Computation*, **2014**, 10, 816-24	6.4	39
91	From four- to six-coordinated silica: Transformation pathways from metadynamics. *Physical Review B*, **2007**, 76,	3.3	39
90	A Strategy to Suppress Phonon Transport in Molecular Junctions Using Stacked Systems. *Journal of Physical Chemistry C*, **2017**, 121, 7175-7182	3.8	38

89	Native surface oxide turns alloyed silicon membranes into nanophononic metamaterials with ultralow thermal conductivity. *Physical Review B*, **2017**, 95,	3.3	38
88	Electron-phonon interaction and thermal boundary resistance at the crystal-amorphous interface of the phase change compound GeTe. *Journal of Applied Physics*, **2015**, 117, 015304	2.5	38
87	Influence of temperature and anisotropic pressure on the phase transitions in alpha-cristobalite. *Physical Review Letters*, **2008**, 100, 165502	7.4	36
86	Photoelasticity of sodium silicate glass from first principles. *Physical Review B*, **2004**, 70,	3.3	36
85	Quasi-Ballistic Thermal Transport Across MoS Thin Films. *Nano Letters*, **2019**, 19, 2434-2442	11.5	34
84	Interaction of charged amino-acid side chains with ions: an optimization strategy for classical force fields. *Journal of Physical Chemistry B*, **2014**, 118, 3960-72	3.4	33
83	DFT research on the dehydroxylation reaction of pyrophyllite 1. First-principle molecular dynamics simulations. *Journal of Physical Chemistry B*, **2008**, 112, 7051-60	3.4	33
82	Toward Hamiltonian Adaptive QM/MM: Accurate Solvent Structures Using Many-Body Potentials. *Journal of Chemical Theory and Computation*, **2016**, 12, 3441-8	6.4	31
81	Nucleation of tetrahedral solids: A molecular dynamics study of supercooled liquid silicon. *Journal of Chemical Physics*, **2009**, 131, 224519	3.9	29
80	Electronic effects in the IR spectrum of water under confinement. *Journal of Physical Chemistry B*, **2009**, 113, 4170-5	3.4	28
79	High Seebeck Coefficient and Unusually Low Thermal Conductivity Near Ambient Temperatures in Layered Compound Yb2EuxCdSb2. *Chemistry of Materials*, **2018**, 30, 484-493	9.6	27
78	Cluster expansion and optimization of thermal conductivity in SiGe nanowires. *Physical Review B*, **2010**, 81,	3.3	27
77	Probing properties of water under confinement: infrared spectra. *Nano Letters*, **2008**, 8, 2959-62	11.5	27
76	Combined Experimental and Theoretical Investigation of Heating Rate on Growth of Iron Oxide Nanoparticles. *Chemistry of Materials*, **2017**, 29, 9648-9656	9.6	26
75	Decisive role of nuclear quantum effects on surface mediated water dissociation at finite temperature. *Journal of Chemical Physics*, **2018**, 148, 102320	3.9	26
74	Trends in the Adsorption and Dissociation of Water Clusters on Flat and Stepped Metallic Surfaces. *Journal of Physical Chemistry C*, **2014**, 118, 29990-29998	3.8	26
73	Adsorption of Dichlorobenzene on Au and Pt Stepped Surfaces Using van der Waals Density Functional Theory. *Journal of Physical Chemistry C*, **2012**, 116, 20409-20416	3.8	25
72	Ab initio investigation of the melting line of nitrogen at high pressure. *Physical Review B*, **2010**, 82,	3.3	25

71	Photoelasticity of crystalline and amorphous silica from first principles. *Physical Review B*, **2003**, 68,	3.3	25
70	A unified framework for force-based and energy-based adaptive resolution simulations. *Europhysics Letters*, **2014**, 108, 30007	1.6	24
69	Structure and Dynamics of the Quasi-Liquid Layer at the Surface of Ice from Molecular Simulations. *Journal of Physical Chemistry C*, **2018**, 122, 24780-24787	3.8	23
68	Flexible and Ultrasoft Inorganic 1D Semiconductor and Heterostructure Systems Based on SnIP. *Advanced Functional Materials*, **2019**, 29, 1900233	15.6	22
67	Thermal conductivity of one-, two- and three-dimensional sp2carbon. *New Journal of Physics*, **2013**, 15, 105019	2.9	21
66	Bimodal Grain-Size Scaling of Thermal Transport in Polycrystalline Graphene from Large-Scale Molecular Dynamics Simulations. *Nano Letters*, **2017**, 17, 5919-5924	11.5	21
65	Thermal transport in free-standing silicon membranes: influence of dimensional reduction and surface nanostructures. *European Physical Journal B*, **2015**, 88, 1	1.2	20
64	Ab initio simulation of photoinduced transformation of small rings in amorphous silica. *Physical Review B*, **2005**, 71,	3.3	19
63	From Classical to Quantum and Back: A Hamiltonian Scheme for Adaptive Multiresolution Classical/Path-Integral Simulations. *Journal of Chemical Theory and Computation*, **2016**, 12, 3030-9	6.4	19
62	Strongly tunable anisotropic thermal transport in MoS 2 by strain and lithium intercalation: first-principles calculations. *2D Materials*, **2019**, 6, 025033	5.9	19
61	Tuning the Adsorption of Aromatic Molecules on Platinum via Halogenation. *Journal of Physical Chemistry C*, **2014**, 118, 6235-6241	3.8	18
60	Atomistic calculation of the thermal conductance of large scale bulk-nanowire junctions. *Physical Review B*, **2011**, 84,	3.3	17
59	DFT research on the dehydroxylation reaction of pyrophyllite 2. Characterization of reactants, intermediates, and transition states along the reaction path. *Journal of Physical Chemistry A*, **2008**, 112, 6373-83	2.8	17
58	III-V Clathrate Semiconductors with Outstanding Hole Mobility: CsInSb and GaSb (= Cs, Rb). *Journal of the American Chemical Society*, **2020**, 142, 2031-2041	16.4	16
57	Structural Complexity and High Thermoelectric Performance of the Zintl Phase: Yb21Mn4Sb18. *Chemistry of Materials*, **2019**, 31, 8076-8086	9.6	15
56	Accurate and general treatment of electrostatic interaction in Hamiltonian adaptive resolution simulations. *European Physical Journal: Special Topics*, **2016**, 225, 1505-1526	2.3	15
55	Simulating Energy Relaxation in Pump-Probe Vibrational Spectroscopy of Hydrogen-Bonded Liquids. *Journal of Chemical Theory and Computation*, **2017**, 13, 1284-1292	6.4	14
54	Efficient thermal diode with ballistic spacer. *Physical Review E*, **2018**, 97, 030101	2.4	14

53	Exploring the rehydroxylation reaction of pyrophyllite by ab initio molecular dynamics. *Journal of Physical Chemistry B*, **2010**, 114, 7593-601	3.4	14
52	Effect of van der Waals interactions on the chemisorption and physisorption of phenol and phenoxy on metal surfaces. *Journal of Chemical Physics*, **2016**, 145, 104701	3.9	14
51	Theoretical investigation of methane under pressure. *Journal of Chemical Physics*, **2009**, 130, 164520	3.9	13
50	Migration of positively charged defects in □quartz. *Physical Review B*, **2007**, 76,	3.3	13
49	Direct observation of ultrafast hydrogen bond strengthening in liquid water. *Nature*, **2021**, 596, 531-535	50.4	13
48	The interplay between surface-water and hydrogen bonding in a water adlayer on Pt(111) and Ag(111). *Journal of Physics Condensed Matter*, **2007**, 19, 242101	1.8	12
47	Atomistic simulations of thermal conductivity in GeTe nanowires. *Journal Physics D: Applied Physics*, **2020**, 53, 054001	3	12
46	Transferability of neural network potentials for varying stoichiometry: Phonons and thermal conductivity of MnxGey compounds. *Journal of Applied Physics*, **2020**, 127, 244901	2.5	12
45	Molecular Mechanism of Crystal Growth Inhibition at the Calcium Oxalate/Water Interfaces. *Journal of Physical Chemistry C*, **2016**, 120, 4410-4417	3.8	11
44	Enhanced thermoelectric performance of two dimensional MS2 (M□□Mo, W) through phase engineering. *Journal of Materiomics*, **2018**, 4, 329-337	6.7	11
43	Atomistic simulations of heat transport in real-scale silicon nanowire devices. *Applied Physics Letters*, **2012**, 100, 223107	3.4	11
42	Optimal thickness of silicon membranes to achieve maximum thermoelectric efficiency: A first principles study. *Applied Physics Letters*, **2016**, 109, 053902	3.4	11
41	Thermal transport across graphene step junctions. *2D Materials*, **2019**, 6, 011005	5.9	11
40	Simulation of atomic force microscopy of fractal nanostructured carbon films. *Europhysics Letters*, **2001**, 54, 72-76	1.6	10
39	Hierarchical thermoelectrics: crystal grain boundaries as scalable phonon scatterers. *Nanoscale*, **2016**, 8, 3729-38	7.7	9
38	Molecular simulation of oligo-glutamates in a calcium-rich aqueous solution: insights into peptide-induced polymorph selection. *CrystEngComm*, **2015**, 17, 6863-6867	3.3	8
37	Proton Wires via One-Dimensional Water Chains Adsorbed on Metallic Steps. *Journal of Chemical Theory and Computation*, **2011**, 7, 2681-4	6.4	8
36	Thermal transport in amorphous small organic materials: a mechanistic study. *Physical Chemistry Chemical Physics*, **2020**, 22, 3058-3065	3.6	8

35	Synergistic impeding of phonon transport through resonances and screw dislocations. *Physical Review B*, **2021**, 103,	3.3	8
34	Energy Relaxation and Thermal Diffusion in Infrared Pump-Probe Spectroscopy of Hydrogen-Bonded Liquids. *Journal of Physical Chemistry Letters*, **2019**, 10, 3447-3452	6.4	7
33	Water Release from Pyrophyllite during the Dehydroxylation Process Explored by Quantum Mechanical Simulations. *Journal of Physical Chemistry C*, **2013**, 117, 7526-7532	3.8	7
32	Dissociative Adsorption of Water at (211) Stepped Metallic Surfaces by First-Principles Simulations. *Journal of Physical Chemistry C*, **2017**, 121, 16783-16791	3.8	7
31	Non-equilibrium dynamics and structure of interfacial ice. *Chemical Physics Letters*, **2006**, 426, 115-119	2.5	7
30	Elastic moduli of nanostructured carbon films. *Physical Review B*, **2004**, 70,	3.3	7
29	Anisotropic In-Plane Phonon Transport in Silicon Membranes Guided by Nanoscale Surface Resonators. *Physical Review Applied*, **2020**, 14,	4.3	7
28	Adsorption of polyiodobenzene molecules on the Pt(111) surface using van der Waals density functional theory. *Surface Science*, **2016**, 644, 113-121	1.8	6
27	Practical algorithms to facilitate large-scale first-principles molecular dynamics. *Journal of Physics: Conference Series*, **2009**, 180, 012074	0.3	6
26	Ultrahigh Convergent Thermal Conductivity of Carbon Nanotubes from Comprehensive Atomistic Modeling. *Physical Review Letters*, **2021**, 127, 025902	7.4	6
25	Advances in the optimization of silicon-based thermoelectrics: a theory perspective. *Current Opinion in Green and Sustainable Chemistry*, **2019**, 17, 35-41	7.9	5
24	Freezing point depression in model Lennard-Jones solutions. *Molecular Physics*, **2015**, 113, 2725-2734	1.7	5
23	Nanofriction Behavior of Cluster-Assembled Carbon Films. *Journal of Nanoscience and Nanotechnology*, **2002**, 2, 637-643	1.3	5
22	Photodecay of guaiacol is faster in ice, and even more rapid on ice, than in aqueous solution. *Environmental Sciences: Processes and Impacts*, **2020**, 22, 1666-1677	4.3	5
21	Beating the Thermal Conductivity Alloy Limit Using Long-Period Compositionally Graded Si1−xGex Superlattices. *Journal of Physical Chemistry C*, **2020**, 124, 19864-19872	3.8	5
20	Solid Solution YbCaCdSb: Structure, Thermoelectric Properties, and Quality Factor. *Inorganic Chemistry*, **2021**, 60, 13596-13606	5.1	5
19	Simulation of the grafting of organosilanes at the surface of dry amorphous silica. *Journal of Physics Condensed Matter*, **2008**, 20, 224011	1.8	4
18	Efficient anharmonic lattice dynamics calculations of thermal transport in crystalline and disordered solids. *Journal of Applied Physics*, **2020**, 128, 135104	2.5	4

17	Selective adsorption of a supramolecular structure on flat and stepped gold surfaces. *Surface Science*, **2018**, 670, 44-50	1.8	3
16	Atomic scale characterization of nanostructured a-C:H films. *European Physical Journal B*, **2002**, 27, 335-340	1.2	3
15	Carbon dioxide, bicarbonate and carbonate ions in aqueous solutions under deep Earth conditions. *Physical Chemistry Chemical Physics*, **2020**, 22, 10717-10725	3.6	3
14	Bathochromic Shift in the UV-Visible Absorption Spectra of Phenols at Ice Surfaces: Insights from First-Principles Calculations. *Journal of Physical Chemistry A*, **2020**, 124, 9288-9298	2.8	3
13	Mode localization and suppressed heat transport in amorphous alloys. *Physical Review B*, **2021**, 103,	3.3	3
12	Simulation of Dimensionality Effects in Thermal Transport. *Lecture Notes in Physics*, **2016**, 275-304	0.8	2
11	Ab initio characterization of graphene nanoribbons and their polymer precursors. *Journal of Physics Condensed Matter*, **2012**, 24, 104023	1.8	2
10	Unprecedented superstructure in the type I family of clathrates. *Chemical Communications*, **2021**,	5.8	2
9	Covalent Cluster-Assembled Carbon Solids **2001**, 89-126		2
8	Thermal Transport: Overview **2018**, 1-11		2
7	Nanofriction behavior of cluster-assembled carbon films. *Journal of Nanoscience and Nanotechnology*, **2002**, 2, 637-43	1.3	1
6	Engineering Thermal Transport across Layered Graphene-MoS Superlattices. *ACS Nano*, **2021**,	16.7	1
5	Mn-intercalated MoSe under pressure: Electronic structure and vibrational characterization of a dilute magnetic semiconductor. *Journal of Chemical Physics*, **2020**, 153, 124701	3.9	1
4	Evolution of structure and transport properties of the Ba8Cu16P30 clathrate-I framework with the introduction of Ga. *Applied Physics Letters*, **2022**, 120, 191901	3.4	0
3	Enhanced photodegradation of dimethoxybenzene isomers in/on ice compared to in aqueous solution. *Atmospheric Chemistry and Physics*, **2022**, 22, 5943-5959	6.8	0
2	Hybrid Materials: Flexible and Ultrasoft Inorganic 1D Semiconductor and Heterostructure Systems Based on SnIP (Adv. Funct. Mater. 18/2019). *Advanced Functional Materials*, **2019**, 29, 1970120	15.6	
1	Thermal Transport: Overview **2020**, 723-733		