Gabriele Cesare Sosso

List of Publications by Year
in descending order

47 papers	3,250 citations	218677 26 h-index	214800 47 g-index
47 all docs	47 docs citations	47 times ranked	3492 citing authors

#	Article	IF	Citations
1	Promoting transparency and reproducibility in enhanced molecular simulations. Nature Methods, 2019, 16, 670-673.	19.0	655
2	Crystal Nucleation in Liquids: Open Questions and Future Challenges in Molecular Dynamics Simulations. Chemical Reviews, 2016, 116, 7078-7116.	47.7	635
3	Neural network interatomic potential for the phase change material GeTe. Physical Review B, 2012, 85, .	3.2	198
4	The Many Faces of Heterogeneous Ice Nucleation: Interplay Between Surface Morphology and Hydrophobicity. Journal of the American Chemical Society, 2015, 137, 13658-13669.	13.7	182
5	Fast Crystallization of the Phase Change Compound GeTe by Large-Scale Molecular Dynamics Simulations. Journal of Physical Chemistry Letters, 2013, 4, 4241-4246.	4.6	133
6	Raman spectra of cubic and amorphous Ge<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow /><mml:mrow><mml:mn>2</mml:mn></mml:mrow></mml:msub></mml:mrow></mml:math>Sb<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow /><mml:mrow><mml:mn>2</mml:mn></mml:mro	3.2	106
7	Analyzing and Driving Cluster Formation in Atomistic Simulations. Journal of Chemical Theory and Computation, 2017, 13, 1317-1327.	5.3	82
8	Ice is born in low-mobility regions of supercooled liquid water. Proceedings of the National Academy of Sciences of the United States of America, 2019, 116, 2009-2014.	7.1	79
9	Microscopic Mechanism and Kinetics of Ice Formation at Complex Interfaces: Zooming in on Kaolinite. Journal of Physical Chemistry Letters, 2016, 7, 2350-2355.	4.6	77
10	Thermal transport in phase-change materials from atomistic simulations. Physical Review B, 2012, 86, .	3.2	75
11	Breakdown of Stokesâ€“Einstein relation in the supercooled liquid state of phase change materials. Physica Status Solidi (B): Basic Research, 2012, 249, 1880-1885.	1.5	75
12	Understanding the thermal properties of amorphous solids using machine-learning-based interatomic potentials. Molecular Simulation, 2018, 44, 866-880.	2.0	69
13	The atomistic details of the ice recrystallisation inhibition activity of PVA. Nature Communications, 2021, 12, 1323.	12.8	62
14	Dynamical Heterogeneity in the Supercooled Liquid State of the Phase Change Material GeTe. Journal of Physical Chemistry B, 2014, 118, 13621-13628.	2.6	57
15	Vibrational properties of hexagonal Ge₂Sb₂Te₅from first principles. Journal of Physics Condensed Matter, 2009, 21, 245401.	1.8	55
16	Pre-critical fluctuations and what they disclose about heterogeneous crystal nucleation. Nature Communications, 2017, 8, 2257.	12.8	55
17	Ice formation on kaolinite: Insights from molecular dynamics simulations. Journal of Chemical Physics, 2016, 145, 211927.	3.0	53
18	Unravelling the origins of ice nucleation on organic crystals. Chemical Science, 2018, 9, 8077-8088.	7.4	43

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19	Atomistic Simulations of the Crystallization and Aging of GeTe Nanowires. Journal of Physical Chemistry C, 2017, 121, 23827-23838.	3.1	42
20	Electron-phonon interaction and thermal boundary resistance at the crystal-amorphous interface of the phase change compound GeTe. Journal of Applied Physics, 2015, 117, .	2.5	41
21	Is High-Density Amorphous Ice Simply a â€œDerailedâ€•State along the Ice I to Ice IV Pathway?. Journal of Physical Chemistry Letters, 2017, 8, 1645-1650.	4.6	38
22	Combining high-resolution scanning tunnelling microscopy and first-principles simulations to identify halogen bonding. Nature Communications, 2020, 11, 2103.	12.8	34
23	High and low density patches in simulated liquid water. Journal of Chemical Physics, 2018, 149, 204507.	3.0	33
24	The role of the umbrella inversion mode in proton diffusion. Chemical Physics Letters, 2014, 599, 133-138.	2.6	31
25	The seven deadly sins: When computing crystal nucleation rates, the devil is in the details. Journal of Chemical Physics, 2021, 155, 040901.	3.0	29
26	Heterogeneous Crystallization of the Phase Change Material GeTe via Atomistic Simulations. Journal of Physical Chemistry C, 2015, 119, 6428-6434.	3.1	28
27	A minimalistic cyclic ice-binding peptide from phage display. Nature Communications, 2021, 12, 2675.	12.8	26
28	On the Role of Nonspherical Cavities in Short Length-Scale Density Fluctuations in Water. Journal of Physical Chemistry A, 2017, 121, 370-380.	2.5	24
29	Harnessing machine learning potentials to understand the functional properties of phase-change materials. MRS Bulletin, 2019, 44, 705-709.	3.5	24
30	Microscopic Kinetics Pathway of Salt Crystallization in Graphene Nanocapillaries. Physical Review Letters, 2021, 126, 136001.	7.8	22
31	Heterogeneous seeded molecular dynamics as a tool to probe the ice nucleating ability of crystalline surfaces. Journal of Chemical Physics, 2018, 149, 072327.	3.0	20
32	Atomistic simulations of thermal conductivity in GeTe nanowires. Journal Physics D: Applied Physics, 2020, 53, 054001.	2.8	20
33	Enhancement of Macromolecular Ice Recrystallization Inhibition Activity by Exploiting Depletion Forces. ACS Macro Letters, 2019, 8, 1063-1067.	4.8	19
34	Priming effects in the crystallization of the phase change compound GeTe from atomistic simulations. Faraday Discussions, 2019, 213, 287-301.	3.2	18
35	Ice Recrystallization Inhibition by Amino Acids: The Curious Case of Alpha- and Beta-Alanine. Journal of Physical Chemistry Letters, 2022, 13, 2237-2244.	4.6	17
36	Insights into the Emerging Networks of Voids in Simulated Supercooled Water. Journal of Physical Chemistry B, 2020, 124, 2180-2190.	2.6	14

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37	Communication: Truncated non-bonded potentials can yield unphysical behavior in molecular dynamics simulations of interfaces. Journal of Chemical Physics, 2017, 147, 121102.	3.0	13
38	GrÃ¼neisen parameters and thermal conductivity in the phase change compound GeTe. Journal of Computational Electronics, 2017, 16, 997-1002.	2.5	13
39	The role of structural order in heterogeneous ice nucleation. Chemical Science, 2022, 13, 5014-5026.	7.4	10
40	Minimalistic ice recrystallisation inhibitors based on phenylalanine. Chemical Communications, 2022, 58, 7658-7661.	4.1	9
41	Electronâ€“phonon interaction and thermal boundary resistance at the interfaces of Ge₂Sb₂Te₅with metals and dielectrics. Journal of Physics Condensed Matter, 2015, 27, 175009.	1.8	8
42	Less may be more: an informed reflection on molecular descriptors for drug design and discovery. Molecular Systems Design and Engineering, 2020, 5, 317-329.	3.4	8
43	Density functional simulations of hexagonal Ge2Sb2Te5at high pressure. Physical Review B, 2013, 87, .	3.2	5
44	Recovering local structure information from high-pressure total scattering experiments. Journal of Applied Crystallography, 2021, 54, 1546-1554.	4.5	5
45	How do interfaces alter the dynamics of supercooled water?. Nanoscale, 2022, 14, 4254-4262.	5.6	4
46	Lipid bilayers as potential ice nucleating agents. Physical Chemistry Chemical Physics, 2022, 24, 6476-6491.	2.8	3
47	Functional Properties of Phase Change Materials from Atomistic Simulations. Springer Series in Materials Science, 2015, , 415-440.	0.6	1