Valentina Tozzini

List of Publications by Year
in descending order

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87	6,935	136885	58549
papers	citations	32 h-index	82 g-index

92	92	92	10902
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Graphene, related two-dimensional crystals, and hybrid systems for energy conversion and storage. Science, 2015, 347, 1246501.	6.0	2,925
2	Coarse-grained models for proteins. Current Opinion in Structural Biology, 2005, 15, 144-150.	2.6	773
3	Prospects for hydrogen storage in graphene. Physical Chemistry Chemical Physics, 2013, 15, 80-89.	1.3	469
4	Reversible Hydrogen Storage by Controlled Buckling of Graphene Layers. Journal of Physical Chemistry C, 2011, 115, 25523-25528.	1.5	159
5	Exploring Global Motions and Correlations in the Ribosome. Biophysical Journal, 2005, 89, 1455-1463.	0.2	131
6	Multiscale Modeling of Proteins. Accounts of Chemical Research, 2010, 43, 220-230.	7.6	127
7	Influence of Graphene Curvature on Hydrogen Adsorption: Toward Hydrogen Storage Devices. Journal of Physical Chemistry C, 2013, 117, 11506-11513.	1.5	125
8	A coarse grained model for the dynamics of flap opening in HIV-1 protease. Chemical Physics Letters, 2005, 413, 123-128.	1.2	123
9	Flap opening dynamics in HIV-1 protease explored with a coarse-grained model. Journal of Structural Biology, 2007, 157, 606-615.	1.3	113
10	The Influence of Macromolecular Crowding on HIV-1 Protease Internal Dynamics. Journal of the American Chemical Society, 2006, 128, 6006-6007.	6.6	96
11	Minimalist models for proteins: a comparative analysis. Quarterly Reviews of Biophysics, 2010, 43, 333-371.	2.4	96
12	Relationship between structure and optical properties in green fluorescent proteins: a quantum mechanical study of the chromophore environment. Chemical Physics, 2004, 298, 17-28.	0.9	87
13	Gated Binding of Ligands to HIV-1 Protease: Brownian Dynamics Simulations in a Coarse-Grained Model. Biophysical Journal, 2006, 90, 3880-3885.	0.2	80
14	Coarseâ€grained force field for the nucleosome from selfâ€consistent multiscaling. Journal of Computational Chemistry, 2008, 29, 1429-1439.	1.5	77
15	HIV-1 Protease Substrate Binding and Product Release Pathways Explored with Coarse-Grained Molecular Dynamics. Biophysical Journal, 2007, 92, 4179-4187.	0.2	74
16	Graphene-based technologies for energy applications, challenges and perspectives. 2D Materials, 2015, 2, 030204.	2.0	74
17	Diffusion within the Cytoplasm: A Mesoscale Model of Interacting Macromolecules. Biophysical Journal, 2014, 107, 2579-2591.	0.2	73
18	GCN5-dependent acetylation of HIV-1 integrase enhances viral integration. Retrovirology, 2010, 7, 18.	0.9	70

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19	Binding Pathways of Ligands to HIV-1 Protease: Coarse-grained and Atomistic Simulations. Chemical Biology and Drug Design, 2007, 69, 5-13.	1.5	67
20	Mapping All-Atom Models onto One-Bead Coarse-Grained Models:Â General Properties and Applications to a Minimal Polypeptide Model. Journal of Chemical Theory and Computation, 2006, 2, 667-673.	2.3	64
21	Ab Initio Molecular Dynamics of the Green Fluorescent Protein (GFP) Chromophore:Â An Insight into the Photoinduced Dynamics of Green Fluorescent Proteins. Journal of Physical Chemistry B, 2001, 105, 5797-5803.	1.2	60
22	Superlubricity of epitaxial monolayer WS2 on graphene. Nano Research, 2018, 11, 5946-5956.	5.8	58
23	Photoreversible Dark State in a Tristable Green Fluorescent Protein Variant. Journal of Physical Chemistry B, 2003, 107, 1679-1684.	1.2	57
24	Coherent Dynamics of Photoexcited Green Fluorescent Proteins. Physical Review Letters, 2001, 86, 3439-3442.	2.9	56
25	Variation of spectral, structural, and vibrational properties within the intrinsically fluorescent proteins family: A density functional study. Journal of Computational Chemistry, 2007, 28, 2366-2377.	1.5	47
26	Molecular dynamics simulations of enhanced green fluorescent proteins: Effects of F64L, S65T and T203Y mutations on the ground-state proton equilibria. Proteins: Structure, Function and Bioinformatics, 2003, 51, 378-389.	1.5	46
27	Raman Study of Chromophore States in Photochromic Fluorescent Proteins. Journal of the American Chemical Society, 2009, 131, 96-103.	6.6	41
28	Electronic structure and Peierls instability in graphene nanoribbons sculpted in graphane. Physical Review B, 2010, 81, .	1.1	40
29	Nano-Scale Corrugations in Graphene: A Density Functional Theory Study of Structure, Electronic Properties and Hydrogenation. Journal of Physical Chemistry C, 2015, 119, 7900-7910.	1.5	39
30	Electronic properties of single-layer tungsten disulfide on epitaxial graphene on silicon carbide. Nanoscale, 2017, 9, 16412-16419.	2.8	39
31	Supercoiling and Local Denaturation of Plasmids with a Minimalist DNA Model. Journal of Physical Chemistry B, 2008, 112, 13197-13200.	1.2	37
32	Fullerene-like IIIâ^'V Clusters:Â A Density Functional Theory Prediction. Journal of Physical Chemistry B, 2001, 105, 12477-12480.	1.2	34
33	Multiscale modeling of proteins interaction with functionalized nanoparticles. Current Opinion in Colloid and Interface Science, 2019, 41, 66-73.	3.4	34
34	Spontaneous Formation and Stability of Small GaP Fullerenes. Physical Review Letters, 2000, 85, 4554-4557.	2.9	31
35	The low frequency vibrational modes of green fluorescent proteins. Chemical Physics, 2003, 287, 33-42.	0.9	31
36	Increasing the active surface of titanium islands on graphene by nitrogen sputtering. Applied Physics Letters, 2015, 106, .	1.5	31

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37	Complexes of HIVâ€1 integrase with HAT proteins: Multiscale models, dynamics, and hypotheses on allosteric sites of inhibition. Proteins: Structure, Function and Bioinformatics, 2009, 76, 946-958.	1.5	29
38	Evolutionary Algorithm in the Optimization of a Coarse-Grained Force Field. Journal of Chemical Theory and Computation, 2013, 9, 4874-4889.	2.3	28
39	Hydrogen Storage in Rippled Graphene: Perspectives from Multi-Scale Simulations. Frontiers in Materials, 2015, 2, .	1.2	22
40	The Chromophore of asFP595:Â A Theoretical Study. Journal of Physical Chemistry B, 2006, 110, 9348-9353.	1.2	21
41	Revealing the Multibonding State between Hydrogen and Graphene-Supported Ti Clusters. Journal of Physical Chemistry C, 2016, 120, 12974-12979.	1.5	21
42	Cisâ€“trans photoisomerization of the chromophore in the green fluorescent protein variant E2GFP: A molecular dynamics study. Chemical Physics, 2006, 323, 358-368.	0.9	20
43	A Minimalist Model of Protein Diffusion and Interactions: The Green Fluorescent Protein within the Cytoplasm. Macromolecules, 2013, 46, 8311-8322.	2.2	20
44	Intrinsic structural and electronic properties of the Buffer Layer on Silicon Carbide unraveled by Density Functional Theory. Scientific Reports, 2018, 8, 13097.	1.6	20
45	Multistable Rippling of Graphene on SiC: A Density Functional Theory Study. Journal of Physical Chemistry C, 2016, 120, 7670-7677.	1.5	17
46	Engineering 3D Graphene-Based Materials: State of the Art and Perspectives. Molecules, 2020, 25, 339.	1.7	15
47	Minimalist models for biopolymers: Open problems, latest advances and perspectives. , 2012, , .		14
48	Atomic and electronic structure of Si dangling bonds in quasi-free-standing monolayer graphene. Nano Research, 2018, 11, 864-873.	5.8	14
49	A Multi-Scaleâ€“Multi-Stable Model for the Rhodopsin Photocycle. Molecules, 2014, 19, 14961-14978.	1.7	13
50	From the Buffer Layer to Graphene on Silicon Carbide: Exploring Morphologies by Computer Modeling. Frontiers in Materials, 2019, 6, .	1.2	13
51	Minimalist Model for the Dynamics of Helical Polypeptides: A Statistic-Based Parametrization. Journal of Chemical Theory and Computation, 2014, 10, 3885-3895.	2.3	12
52	Water splitting of hydrogen chemisorbed in graphene oxide dynamically evolves into a graphane lattice. Carbon, 2019, 153, 234-241.	5.4	12
53	Covalent organic functionalization of graphene nanosheets and reduced graphene oxidevia1,3-dipolar cycloaddition of azomethine ylide. Nanoscale Advances, 2021, 3, 5841-5852.	2.2	11
54	Low-Resolution Models for the Interaction Dynamics of Coated Gold Nanoparticles with Î²2-microglobulin. International Journal of Molecular Sciences, 2019, 20, 3866.	1.8	10

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55	Vibrational and elastic properties of the hot solid related to the static and dynamic structure of the liquid within density functional theory. The Philosophical Magazine: Physics of Condensed Matter B, Statistical Mechanics, Electronic, Optical and Magnetic Properties, 1994, 69, 833-848.	0.6	9
56	Lattice vibrations and elastic constants of three- and two-dimensional quantal Wigner crystals near melting. Journal of Physics Condensed Matter, 1996, 8, 8121-8136.	0.7	9
57	Vibrational Properties of DsRed Model Chromophores. ChemPhysChem, 2005, 6, 1786-1788.	1.0	9
58	Orientational Disorder and Melting Transition: Phenomenology and Modelling with Relevance to Solid Halogens and H2. Physics and Chemistry of Liquids, 1999, 37, 185-191.	0.4	8
59	SecStAnT: secondary structure analysis tool for data selection, statistics and models building. Bioinformatics, 2014, 30, 668-674.	1.8	8
60	Editorial: Multiscale Modeling From Macromolecules to Cell: Opportunities and Challenges of Biomolecular Simulations. Frontiers in Molecular Biosciences, 2020, 7, 194.	1.6	8
61	Unraveling localized states in quasi free standing monolayer graphene by means of Density Functional Theory. Carbon, 2018, 130, 466-474.	5.4	7
62	Vacancy formation energy in the quantal crystals of the two helium isotopes. Philosophical Magazine Letters, 1997, 76, 377-382.	0.5	6
63	Genetic Algorithm Optimization of Force Field Parameters: Application to a Coarse-Grained Model of RNA. Lecture Notes in Computer Science, 2011, , 147-152.	1.0	6
64	Structural Transition States Explored With Minimalist Coarse Grained Models: Applications to Calmodulin. Frontiers in Molecular Biosciences, 2019, 6, 104.	1.6	6
65	Vibrational and Elastic Properties of the Wigner Electron Lattice Near Melting. Europhysics Letters, 1993, 23, 433-438.	0.7	5
66	Optimization of Analytical Potentials for Coarse-Grained Biopolymer Models. Journal of Physical Chemistry B, 2016, 120, 8571-8579.	1.2	5
67	Building Minimalist Models for Functionalized Metal Nanoparticles. Frontiers in Molecular Biosciences, 2019, 6, 50.	1.6	5
68	In silico design, building and gas adsorption of nano-porous graphene scaffolds. Nanotechnology, 2021, 32, 045704.	1.3	5
69	Viscoelastic Model for the Transition from Normal to Fast Sound in Water. Physics and Chemistry of Liquids, 1996, 33, 191-198.	0.4	4
70	Lattice vibrations and elastic constants of crystalline and near low-temperature melting. Physica B: Condensed Matter, 1999, 262, 369-380.	1.3	4
71	One-Photon and Two-Photon Excitation of Fluorescent Proteins. Springer Series on Fluorescence, 2011, , 3-40.	0.8	4
72	Hydrogen transport within graphene multilayers by means of flexural phonons. 2D Materials, 2015, 2, 014009.	2.0	4

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73	III-V semicondutor nanostructures and iontronics: InAs nanowire-based electric double layer field effect transistors. AIP Conference Proceedings, 2019, , .	0.3	4
74	Morphing Graphene-Based Systems for Applications: Perspectives from Simulations. Carbon Nanostructures, 2017, , 87-111.	0.1	4
75	Vibrational and elastic properties of alkali halides near melting. The Philosophical Magazine: Physics of Condensed Matter B, Statistical Mechanics, Electronic, Optical and Magnetic Properties, 1995, 72, 577-588.	0.6	3
76	Lattice dynamics of stage-2 alkali intercalates in graphite. Physica B: Condensed Matter, 1997, 240, 92-97.	1.3	3
77	Dispersion Laws of Collective Excitations in Crystalline and Superfluid 4 He Related via Density-Functional Theory. Europhysics Letters, 1995, 32, 67-72.	0.7	2
78	SDPhound, a Mutual Information-Based Method to Investigate Specificity-Determining Positions. Algorithms, 2009, 2, 764-789.	1.2	2
79	Collective Mode Mining from Molecular Dynamics Simulations: A Comparative Approach. International Journal of Computational Methods, 2018, 15, 1850108.	0.8	2
80	Evolutionary Switches Structural Transitions via Coarse-Grained Models. Journal of Computational Biology, 2020, 27, 189-199.	0.8	2
81	Spontaneous Formation and Stability of GaP Cage Structures: A Theoretical Prediction of a New Fullerene. Materials Research Society Symposia Proceedings, 2001, 675, 1.	0.1	1
82	Vibrational Spectroscopy of Fluorescent Proteins: A Tool to Investigate the Structure of the Chromophore and Its Environment. Springer Series on Fluorescence, 2011, , 133-169.	0.8	1
83	Green Fluorescent Proteins and Their Applications to Cell Biology and Bioelectronics. , 2003, , .		1
84	Deterministic Covalent Organic Functionalization of Monolayer Graphene with 1,3-Dipolar Cycloaddition Via High Resolution Surface Engineering. SSRN Electronic Journal, 0, , .	0.4	1
85	Engineered Green Fluorescence Proteins for Proteomics and Biomolecular Electronic Applications. Macromolecular Symposia, 2004, 218, 283-292.	0.4	0
86	GCN5-dependent acetylation of HIV-1 integrase enhances viral integration. Retrovirology, 2009, 6, P20.	0.9	0
87	One-Bead Coarse-Grained Models for Proteins. , 2008, , 285-298.		0