

Valentina Tozzini

List of Publications by Citations

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The third column is the impact factor (IF) of the journal, and the fourth column is the number of citations of the article.

84
papers

5,914
citations

30
h-index

76
g-index

91
ext. papers

6,550
ext. citations

4.7
avg, IF

6.17
L-index

#	Paper	IF	Citations
84	2D materials. Graphene, related two-dimensional crystals, and hybrid systems for energy conversion and storage. <i>Science</i> , 2015 , 347, 1246501	33.3	2450
83	Coarse-grained models for proteins. <i>Current Opinion in Structural Biology</i> , 2005 , 15, 144-50	8.1	698
82	Prospects for hydrogen storage in graphene. <i>Physical Chemistry Chemical Physics</i> , 2013 , 15, 80-9	3.6	362
81	Reversible Hydrogen Storage by Controlled Buckling of Graphene Layers. <i>Journal of Physical Chemistry C</i> , 2011 , 115, 25523-25528	3.8	133
80	Exploring global motions and correlations in the ribosome. <i>Biophysical Journal</i> , 2005 , 89, 1455-63	2.9	115
79	Multiscale modeling of proteins. <i>Accounts of Chemical Research</i> , 2010 , 43, 220-30	24.3	111
78	A coarse grained model for the dynamics of flap opening in HIV-1 protease. <i>Chemical Physics Letters</i> , 2005 , 413, 123-128	2.5	107
77	Influence of Graphene Curvature on Hydrogen Adsorption: Toward Hydrogen Storage Devices. <i>Journal of Physical Chemistry C</i> , 2013 , 117, 11506-11513	3.8	104
76	Flap opening dynamics in HIV-1 protease explored with a coarse-grained model. <i>Journal of Structural Biology</i> , 2007 , 157, 606-15	3.4	100
75	Minimalist models for proteins: a comparative analysis. <i>Quarterly Reviews of Biophysics</i> , 2010 , 43, 333-717		87
74	The influence of macromolecular crowding on HIV-1 protease internal dynamics. <i>Journal of the American Chemical Society</i> , 2006 , 128, 6006-7	16.4	87
73	Relationship between structure and optical properties in green fluorescent proteins: a quantum mechanical study of the chromophore environment. <i>Chemical Physics</i> , 2004 , 298, 17-28	2.3	86
72	GCN5-dependent acetylation of HIV-1 integrase enhances viral integration. <i>Retrovirology</i> , 2009 , 6, P20	3.6	78
71	Gated binding of ligands to HIV-1 protease: Brownian dynamics simulations in a coarse-grained model. <i>Biophysical Journal</i> , 2006 , 90, 3880-5	2.9	75
70	Coarse-grained force field for the nucleosome from self-consistent multiscaling. <i>Journal of Computational Chemistry</i> , 2008 , 29, 1429-39	3.5	70
69	HIV-1 protease substrate binding and product release pathways explored with coarse-grained molecular dynamics. <i>Biophysical Journal</i> , 2007 , 92, 4179-87	2.9	67
68	Graphene-based technologies for energy applications, challenges and perspectives. <i>2D Materials</i> , 2015 , 2, 030204	5.9	62

67	Binding pathways of ligands to HIV-1 protease: coarse-grained and atomistic simulations. <i>Chemical Biology and Drug Design</i> , 2007 , 69, 5-13	2.9	59
66	GCN5-dependent acetylation of HIV-1 integrase enhances viral integration. <i>Retrovirology</i> , 2010 , 7, 18	3.6	57
65	Mapping all-atom models onto one-bead Coarse Grained Models: general properties and applications to a minimal polypeptide model. <i>Journal of Chemical Theory and Computation</i> , 2006 , 2, 667-673	6.4	57
64	Ab Initio Molecular Dynamics of the Green Fluorescent Protein (GFP) Chromophore: An Insight into the Photoinduced Dynamics of Green Fluorescent Proteins. <i>Journal of Physical Chemistry B</i> , 2001 , 105, 5797-5803	3.4	55
63	Diffusion within the cytoplasm: a mesoscale model of interacting macromolecules. <i>Biophysical Journal</i> , 2014 , 107, 2579-91	2.9	53
62	Photoreversible Dark State in a Tristable Green Fluorescent Protein Variant. <i>Journal of Physical Chemistry B</i> , 2003 , 107, 1679-1684	3.4	53
61	Coherent dynamics of photoexcited green fluorescent proteins. <i>Physical Review Letters</i> , 2001 , 86, 3439-424	4.2	47
60	Variation of spectral, structural, and vibrational properties within the intrinsically fluorescent proteins family: a density functional study. <i>Journal of Computational Chemistry</i> , 2007 , 28, 2366-77	3.5	45
59	Molecular dynamics simulations of enhanced green fluorescent proteins: effects of F64L, S65T and T203Y mutations on the ground-state proton equilibria. <i>Proteins: Structure, Function and Bioinformatics</i> , 2003 , 51, 378-89	4.2	40
58	Electronic structure and Peierls instability in graphene nanoribbons sculpted in graphane. <i>Physical Review B</i> , 2010 , 81,	3.3	39
57	Raman study of chromophore states in photochromic fluorescent proteins. <i>Journal of the American Chemical Society</i> , 2009 , 131, 96-103	16.4	36
56	Supercoiling and local denaturation of plasmids with a minimalist DNA model. <i>Journal of Physical Chemistry B</i> , 2008 , 112, 13197-200	3.4	33
55	Superlubricity of epitaxial monolayer WS ₂ on graphene. <i>Nano Research</i> , 2018 , 11, 5946-5956	10	31
54	Electronic properties of single-layer tungsten disulfide on epitaxial graphene on silicon carbide. <i>Nanoscale</i> , 2017 , 9, 16412-16419	7.7	30
53	Spontaneous formation and stability of small GaP fullerenes. <i>Physical Review Letters</i> , 2000 , 85, 4554-7	7.4	30
52	Nano-Scale Corrugations in Graphene: A Density Functional Theory Study of Structure, Electronic Properties and Hydrogenation. <i>Journal of Physical Chemistry C</i> , 2015 , 119, 7900-7910	3.8	28
51	Fullerene-like III ^V Clusters: A Density Functional Theory Prediction. <i>Journal of Physical Chemistry B</i> , 2001 , 105, 12477-12480	3.4	28
50	Increasing the active surface of titanium islands on graphene by nitrogen sputtering. <i>Applied Physics Letters</i> , 2015 , 106, 083901	3.4	25

49	Complexes of HIV-1 integrase with HAT proteins: multiscale models, dynamics, and hypotheses on allosteric sites of inhibition. <i>Proteins: Structure, Function and Bioinformatics</i> , 2009 , 76, 946-58	4.2	24
48	Evolutionary Algorithm in the Optimization of a Coarse-Grained Force Field. <i>Journal of Chemical Theory and Computation</i> , 2013 , 9, 4874-89	6.4	23
47	The low frequency vibrational modes of green fluorescent proteins. <i>Chemical Physics</i> , 2003 , 287, 33-42	2.3	22
46	The chromophore of asFP595: a theoretical study. <i>Journal of Physical Chemistry B</i> , 2006 , 110, 9348-53	3.4	20
45	Multiscale modeling of proteins interaction with functionalized nanoparticles. <i>Current Opinion in Colloid and Interface Science</i> , 2019 , 41, 66-73	7.6	19
44	Hydrogen Storage in Rippled Graphene: Perspectives from Multi-Scale Simulations. <i>Frontiers in Materials</i> , 2015 , 2,	4	18
43	Intrinsic structural and electronic properties of the Buffer Layer on Silicon Carbide unraveled by Density Functional Theory. <i>Scientific Reports</i> , 2018 , 8, 13097	4.9	17
42	Revealing the Multibonding State between Hydrogen and Graphene-Supported Ti Clusters. <i>Journal of Physical Chemistry C</i> , 2016 , 120, 12974-12979	3.8	16
41	Multistable Rippling of Graphene on SiC: A Density Functional Theory Study. <i>Journal of Physical Chemistry C</i> , 2016 , 120, 7670-7677	3.8	16
40	A Minimalist Model of Protein Diffusion and Interactions: The Green Fluorescent Protein within the Cytoplasm. <i>Macromolecules</i> , 2013 , 46, 8311-8322	5.5	16
39	Cis-trans photoisomerization of the chromophore in the green fluorescent protein variant E2GFP: A molecular dynamics study. <i>Chemical Physics</i> , 2006 , 323, 358-368	2.3	16
38	Atomic and electronic structure of Si dangling bonds in quasi-free-standing monolayer graphene. <i>Nano Research</i> , 2018 , 11, 864-873	10	12
37	Minimalist models for biopolymers: Open problems, latest advances and perspectives 2012 ,		10
36	Engineering 3D Graphene-Based Materials: State of the Art and Perspectives. <i>Molecules</i> , 2020 , 25,	4.8	9
35	Lattice vibrations and elastic constants of three- and two-dimensional quantal Wigner crystals near melting. <i>Journal of Physics Condensed Matter</i> , 1996 , 8, 8121-8136	1.8	9
34	Vibrational and elastic properties of the hot solid related to the static and dynamic structure of the liquid within density functional theory. <i>The Philosophical Magazine: Physics of Condensed Matter B, Statistical Mechanics, Electronic, Optical and Magnetic Properties</i> , 1994 , 69, 833-848		9
33	A multi-scale-multi-stable model for the rhodopsin photocycle. <i>Molecules</i> , 2014 , 19, 14961-78	4.8	8
32	Minimalist Model for the Dynamics of Helical Polypeptides: A Statistic-Based Parametrization. <i>Journal of Chemical Theory and Computation</i> , 2014 , 10, 3885-95	6.4	7

31	Vibrational properties of DsRed model chromophores. <i>ChemPhysChem</i> , 2005 , 6, 1786-8	3.2	7
30	Orientalional Disorder and Melting Transition: Phenomenology and Modelling with Relevance to Solid Halogens and H ₂ . <i>Physics and Chemistry of Liquids</i> , 1999 , 37, 185-191	1.5	7
29	From the Buffer Layer to Graphene on Silicon Carbide: Exploring Morphologies by Computer Modeling. <i>Frontiers in Materials</i> , 2019 , 6,	4	6
28	Unraveling localized states in quasi free standing monolayer graphene by means of Density Functional Theory. <i>Carbon</i> , 2018 , 130, 466-474	10.4	6
27	Water splitting of hydrogen chemisorbed in graphene oxide dynamically evolves into a graphane lattice. <i>Carbon</i> , 2019 , 153, 234-241	10.4	6
26	Genetic Algorithm Optimization of Force Field Parameters: Application to a Coarse-Grained Model of RNA. <i>Lecture Notes in Computer Science</i> , 2011 , 147-152	0.9	6
25	Low-Resolution Models for the Interaction Dynamics of Coated Gold Nanoparticles with α -microglobulin. <i>International Journal of Molecular Sciences</i> , 2019 , 20,	6.3	5
24	SecStAnT: secondary structure analysis tool for data selection, statistics and models building. <i>Bioinformatics</i> , 2014 , 30, 668-74	7.2	5
23	Vacancy formation energy in the quantal crystals of the two helium isotopes. <i>Philosophical Magazine Letters</i> , 1997 , 76, 377-382	1	5
22	Vibrational and Elastic Properties of the Wigner Electron Lattice Near Melting. <i>Europhysics Letters</i> , 1993 , 23, 433-438	1.6	5
21	Viscoelastic Model for the Transition from Normal to Fast Sound in Water. <i>Physics and Chemistry of Liquids</i> , 1996 , 33, 191-198	1.5	4
20	Morphing Graphene-Based Systems for Applications: Perspectives from Simulations. <i>Carbon Nanostructures</i> , 2017 , 87-111	0.6	4
19	III-V semiconductor nanostructures and iontronics: InAs nanowire-based electric double layer field effect transistors 2019 ,		3
18	Hydrogen transport within graphene multilayers by means of flexural phonons. <i>2D Materials</i> , 2015 , 2, 014009	5.9	3
17	Structural Transition States Explored With Minimalist Coarse Grained Models: Applications to Calmodulin. <i>Frontiers in Molecular Biosciences</i> , 2019 , 6, 104	5.6	3
16	One-Photon and Two-Photon Excitation of Fluorescent Proteins. <i>Springer Series on Fluorescence</i> , 2011 , 3-40	0.5	3
15	Lattice dynamics of stage-2 alkali intercalates in graphite. <i>Physica B: Condensed Matter</i> , 1997 , 240, 92-97	2.8	3
14	Lattice vibrations and elastic constants of crystalline 4He and 3He near low-temperature melting. <i>Physica B: Condensed Matter</i> , 1999 , 262, 369-380	2.8	3

13	Vibrational and elastic properties of alkali halides near melting. <i>The Philosophical Magazine: Physics of Condensed Matter B, Statistical Mechanics, Electronic, Optical and Magnetic Properties</i> , 1995 , 72, 577-588		3
12	In silico design, building and gas adsorption of nano-porous graphene scaffolds. <i>Nanotechnology</i> , 2021 , 32, 045704	3.4	3
11	Optimization of Analytical Potentials for Coarse-Grained Biopolymer Models. <i>Journal of Physical Chemistry B</i> , 2016 , 120, 8571-9	3.4	3
10	Covalent organic functionalization of graphene nanosheets and reduced graphene oxide via 1,3-dipolar cycloaddition of azomethine ylide. <i>Nanoscale Advances</i> ,	5.1	3
9	SDPhound, a Mutual Information-Based Method to Investigate Specificity-Determining Positions. <i>Algorithms</i> , 2009 , 2, 764-789	1.8	2
8	Dispersion Laws of Collective Excitations in Crystalline and Superfluid 4 He Related via Density-Functional Theory. <i>Europhysics Letters</i> , 1995 , 32, 67-72	1.6	2
7	Collective Mode Mining from Molecular Dynamics Simulations: A Comparative Approach. <i>International Journal of Computational Methods</i> , 2018 , 15, 1850108	1.1	1
6	Building Minimalist Models for Functionalized Metal Nanoparticles. <i>Frontiers in Molecular Biosciences</i> , 2019 , 6, 50	5.6	1
5	Green Fluorescent Proteins and Their Applications to Cell Biology and Bioelectronics 2003 ,		1
4	Vibrational Spectroscopy of Fluorescent Proteins: A Tool to Investigate the Structure of the Chromophore and Its Environment. <i>Springer Series on Fluorescence</i> , 2011 , 133-169	0.5	0
3	Engineered Green Fluorescence Proteins for Proteomics and Biomolecular Electronic Applications. <i>Macromolecular Symposia</i> , 2004 , 218, 283-292	0.8	
2	Spontaneous Formation and Stability of GaP Cage Structures: A Theoretical Prediction of a New Fullerene. <i>Materials Research Society Symposia Proceedings</i> , 2001 , 675, 1		
1	One-Bead Coarse-Grained Models for Proteins 2008 , 285-298		