Valentina Tozzini

List of Publications by Year in Descending Order

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	In silico design, building and gas adsorption of nano-porous graphene scaffolds. *Nanotechnology*, **2021**, 32, 045704	3.4	3
83	Engineering 3D Graphene-Based Materials: State of the Art and Perspectives. *Molecules*, **2020**, 25,	4.8	9
82	III-V semicondutor nanostructures and iontronics: InAs nanowire-based electric double layer field effect transistors **2019**,		3
81	From the Buffer Layer to Graphene on Silicon Carbide: Exploring Morphologies by Computer Modeling. *Frontiers in Materials*, **2019**, 6,	4	6
80	Low-Resolution Models for the Interaction Dynamics of Coated Gold Nanoparticles with 2-microglobulin. *International Journal of Molecular Sciences*, **2019**, 20,	6.3	5
79	Building Minimalist Models for Functionalized Metal Nanoparticles. *Frontiers in Molecular Biosciences*, **2019**, 6, 50	5.6	1
78	Water splitting of hydrogen chemisorbed in graphene oxide dynamically evolves into a graphane lattice. *Carbon*, **2019**, 153, 234-241	10.4	6
77	Structural Transition States Explored With Minimalist Coarse Grained Models: Applications to Calmodulin. *Frontiers in Molecular Biosciences*, **2019**, 6, 104	5.6	3
76	Multiscale modeling of proteins interaction with functionalized nanoparticles. *Current Opinion in Colloid and Interface Science*, **2019**, 41, 66-73	7.6	19
75	Unraveling localized states in quasi free standing monolayer graphene by means of Density Functional Theory. *Carbon*, **2018**, 130, 466-474	10.4	6
74	Collective Mode Mining from Molecular Dynamics Simulations: A Comparative Approach. *International Journal of Computational Methods*, **2018**, 15, 1850108	1.1	1
73	Superlubricity of epitaxial monolayer WS2 on graphene. *Nano Research*, **2018**, 11, 5946-5956	10	31
72	Atomic and electronic structure of Si dangling bonds in quasi-free-standing monolayer graphene. *Nano Research*, **2018**, 11, 864-873	10	12
71	Intrinsic structural and electronic properties of the Buffer Layer on Silicon Carbide unraveled by Density Functional Theory. *Scientific Reports*, **2018**, 8, 13097	4.9	17
70	Electronic properties of single-layer tungsten disulfide on epitaxial graphene on silicon carbide. *Nanoscale*, **2017**, 9, 16412-16419	7.7	30
69	Morphing Graphene-Based Systems for Applications: Perspectives from Simulations. *Carbon Nanostructures*, **2017**, 87-111	0.6	4
68	Revealing the Multibonding State between Hydrogen and Graphene-Supported Ti Clusters. *Journal of Physical Chemistry C*, **2016**, 120, 12974-12979	3.8	16

67	Multistable Rippling of Graphene on SiC: A Density Functional Theory Study. *Journal of Physical Chemistry C*, **2016**, 120, 7670-7677	3.8	16
66	Optimization of Analytical Potentials for Coarse-Grained Biopolymer Models. *Journal of Physical Chemistry B*, **2016**, 120, 8571-9	3.4	3
65	Hydrogen transport within graphene multilayers by means of flexural phonons. *2D Materials*, **2015**, 2, 014009	5.9	3
64	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	3.8	28
63	Graphene-based technologies for energy applications, challenges and perspectives. *2D Materials*, **2015**, 2, 030204	5.9	62
62	Increasing the active surface of titanium islands on graphene by nitrogen sputtering. *Applied Physics Letters*, **2015**, 106, 083901	3.4	25
61	Hydrogen Storage in Rippled Graphene: Perspectives from Multi-Scale Simulations. *Frontiers in Materials*, **2015**, 2,	4	18
60	2D materials. Graphene, related two-dimensional crystals, and hybrid systems for energy conversion and storage. *Science*, **2015**, 347, 1246501	33.3	2450
59	SecStAnT: secondary structure analysis tool for data selection, statistics and models building. *Bioinformatics*, **2014**, 30, 668-74	7.2	5
58	Minimalist Model for the Dynamics of Helical Polypeptides: A Statistic-Based Parametrization. *Journal of Chemical Theory and Computation*, **2014**, 10, 3885-95	6.4	7
57	A multi-scale-multi-stable model for the rhodopsin photocycle. *Molecules*, **2014**, 19, 14961-78	4.8	8
56	Diffusion within the cytoplasm: a mesoscale model of interacting macromolecules. *Biophysical Journal*, **2014**, 107, 2579-91	2.9	53
55	A Minimalist Model of Protein Diffusion and Interactions: The Green Fluorescent Protein within the Cytoplasm. *Macromolecules*, **2013**, 46, 8311-8322	5.5	16
54	Evolutionary Algorithm in the Optimization of a Coarse-Grained Force Field. *Journal of Chemical Theory and Computation*, **2013**, 9, 4874-89	6.4	23
53	Prospects for hydrogen storage in graphene. *Physical Chemistry Chemical Physics*, **2013**, 15, 80-9	3.6	362
52	Influence of Graphene Curvature on Hydrogen Adsorption: Toward Hydrogen Storage Devices. *Journal of Physical Chemistry C*, **2013**, 117, 11506-11513	3.8	104
51	Minimalist models for biopolymers: Open problems, latest advances and perspectives **2012**,		10
50	Genetic Algorithm Optimization of Force Field Parameters: Application to a Coarse-Grained Model of RNA. *Lecture Notes in Computer Science*, **2011**, 147-152	0.9	6

49	One-Photon and Two-Photon Excitation of Fluorescent Proteins. *Springer Series on Fluorescence*, **2011**, 3-40	0.5	3
48	Reversible Hydrogen Storage by Controlled Buckling of Graphene Layers. *Journal of Physical Chemistry C*, **2011**, 115, 25523-25528	3.8	133
47	Vibrational Spectroscopy of Fluorescent Proteins: A Tool to Investigate the Structure of the Chromophore and Its Environment. *Springer Series on Fluorescence*, **2011**, 133-169	0.5	0
46	Multiscale modeling of proteins. *Accounts of Chemical Research*, **2010**, 43, 220-30	24.3	111
45	Electronic structure and Peierls instability in graphene nanoribbons sculpted in graphane. *Physical Review B*, **2010**, 81,	3.3	39
44	Minimalist models for proteins: a comparative analysis. *Quarterly Reviews of Biophysics*, **2010**, 43, 333-717		87
43	GCN5-dependent acetylation of HIV-1 integrase enhances viral integration. *Retrovirology*, **2010**, 7, 18	3.6	57
42	SDPhound, a Mutual Information-Based Method to Investigate Specificity-Determining Positions. *Algorithms*, **2009**, 2, 764-789	1.8	2
41	Complexes of HIV-1 integrase with HAT proteins: multiscale models, dynamics, and hypotheses on allosteric sites of inhibition. *Proteins: Structure, Function and Bioinformatics*, **2009**, 76, 946-58	4.2	24
40	Raman study of chromophore states in photochromic fluorescent proteins. *Journal of the American Chemical Society*, **2009**, 131, 96-103	16.4	36
39	GCN5-dependent acetylation of HIV-1 integrase enhances viral integration. *Retrovirology*, **2009**, 6, P20	3.6	78
38	Supercoiling and local denaturation of plasmids with a minimalist DNA model. *Journal of Physical Chemistry B*, **2008**, 112, 13197-200	3.4	33
37	Coarse-grained force field for the nucleosome from self-consistent multiscaling. *Journal of Computational Chemistry*, **2008**, 29, 1429-39	3.5	70
36	One-Bead Coarse-Grained Models for Proteins **2008**, 285-298		
35	HIV-1 protease substrate binding and product release pathways explored with coarse-grained molecular dynamics. *Biophysical Journal*, **2007**, 92, 4179-87	2.9	67
34	Variation of spectral, structural, and vibrational properties within the intrinsically fluorescent proteins family: a density functional study. *Journal of Computational Chemistry*, **2007**, 28, 2366-77	3.5	45
33	Binding pathways of ligands to HIV-1 protease: coarse-grained and atomistic simulations. *Chemical Biology and Drug Design*, **2007**, 69, 5-13	2.9	59
32	Flap opening dynamics in HIV-1 protease explored with a coarse-grained model. *Journal of Structural Biology*, **2007**, 157, 606-15	3.4	100

31	Cis□trans photoisomerization of the chromophore in the green fluorescent protein variant E2GFP: A molecular dynamics study. *Chemical Physics*, **2006**, 323, 358-368	2.3	16
30	The influence of macromolecular crowding on HIV-1 protease internal dynamics. *Journal of the American Chemical Society*, **2006**, 128, 6006-7	16.4	87
29	Mapping all-atom models onto one-bead Coarse Grained Models: general properties and applications to a minimal polypeptide model. *Journal of Chemical Theory and Computation*, **2006**, 2, 667-673	6.4	57
28	Gated binding of ligands to HIV-1 protease: Brownian dynamics simulations in a coarse-grained model. *Biophysical Journal*, **2006**, 90, 3880-5	2.9	75
27	The chromophore of asFP595: a theoretical study. *Journal of Physical Chemistry B*, **2006**, 110, 9348-53	3.4	20
26	Exploring global motions and correlations in the ribosome. *Biophysical Journal*, **2005**, 89, 1455-63	2.9	115
25	A coarse grained model for the dynamics of flap opening in HIV-1 protease. *Chemical Physics Letters* , **2005**, 413, 123-128	2.5	107
24	Coarse-grained models for proteins. *Current Opinion in Structural Biology*, **2005**, 15, 144-50	8.1	698
23	Vibrational properties of DsRed model chromophores. *ChemPhysChem*, **2005**, 6, 1786-8	3.2	7
22	Relationship between structure and optical properties in green fluorescent proteins: a quantum mechanical study of the chromophore environment. *Chemical Physics*, **2004**, 298, 17-28	2.3	86
21	Engineered Green Fluorescence Proteins for Proteomics and Biomolecular Electronic Applications. *Macromolecular Symposia*, **2004**, 218, 283-292	0.8	
20	The low frequency vibrational modes of green fluorescent proteins. *Chemical Physics*, **2003**, 287, 33-42	2.3	22
19	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, 378-89	4.2	40
18	Photoreversible Dark State in a Tristable Green Fluorescent Protein Variant. *Journal of Physical Chemistry B*, **2003**, 107, 1679-1684	3.4	53
17	Green Fluorescent Proteins and Their Applications to Cell Biology and Bioelectronics **2003**,		1
16	Ab Initio Molecular Dynamics of the Green Fluorescent Protein (GFP) Chromophore: An Insight into the Photoinduced Dynamics of Green Fluorescent Proteins. *Journal of Physical Chemistry B*, **2001**, 105, 5797-5803	3.4	55
15	Coherent dynamics of photoexcited green fluorescent proteins. *Physical Review Letters*, **2001**, 86, 3439-42	7.4	47
14	Fullerene-like III□V Clusters: A Density Functional Theory Prediction. *Journal of Physical Chemistry B* , **2001**, 105, 12477-12480	3.4	28

13	Spontaneous Formation and Stability of GaP Cage Structures: A Theoretical Prediction of a New Fullerene. *Materials Research Society Symposia Proceedings*, **2001**, 675, 1		
12	Spontaneous formation and stability of small GaP fullerenes. *Physical Review Letters*, **2000**, 85, 4554-7	7.4	30
11	Orientational Disorder and Melting Transition: Phenomenology and Modelling with Relevance to Solid Halogens and H2. *Physics and Chemistry of Liquids*, **1999**, 37, 185-191	1.5	7
10	Lattice vibrations and elastic constants of crystalline 4He and 3He near low-temperature melting. *Physica B: Condensed Matter*, **1999**, 262, 369-380	2.8	3
9	Vacancy formation energy in the quantal crystals of the two helium isotopes. *Philosophical Magazine Letters*, **1997**, 76, 377-382	1	5
8	Lattice dynamics of stage-2 alkali intercalates in graphite. *Physica B: Condensed Matter*, **1997**, 240, 92-97	2.8	3
7	Lattice vibrations and elastic constants of three- and two-dimensional quantal Wigner crystals near melting. *Journal of Physics Condensed Matter*, **1996**, 8, 8121-8136	1.8	9
6	Viscoelastic Model for the Transition from Normal to Fast Sound in Water. *Physics and Chemistry of Liquids*, **1996**, 33, 191-198	1.5	4
5	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		3
4	Dispersion Laws of Collective Excitations in Crystalline and Superfluid 4 He Related via Density-Functional Theory. *Europhysics Letters*, **1995**, 32, 67-72	1.6	2
3	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		9
2	Vibrational and Elastic Properties of the Wigner Electron Lattice Near Melting. *Europhysics Letters*, **1993**, 23, 433-438	1.6	5
1	Covalent organic functionalization of graphene nanosheets and reduced graphene oxide via 1,3-dipolar cycloaddition of azomethine ylide. *Nanoscale Advances*,	5.1	3