

Valentina Tozzini

List of Publications by Year in descending order

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87
papers

6,935
citations

136950

32
h-index

58581

82
g-index

92
all docs

92
docs citations

92
times ranked

10902
citing authors

#	ARTICLE	IF	CITATIONS
1	Graphene, related two-dimensional crystals, and hybrid systems for energy conversion and storage. <i>Science</i> , 2015, 347, 1246501.	12.6	2,925
2	Coarse-grained models for proteins. <i>Current Opinion in Structural Biology</i> , 2005, 15, 144-150.	5.7	773
3	Prospects for hydrogen storage in graphene. <i>Physical Chemistry Chemical Physics</i> , 2013, 15, 80-89.	2.8	469
4	Reversible Hydrogen Storage by Controlled Buckling of Graphene Layers. <i>Journal of Physical Chemistry C</i> , 2011, 115, 25523-25528.	3.1	159
5	Exploring Global Motions and Correlations in the Ribosome. <i>Biophysical Journal</i> , 2005, 89, 1455-1463.	0.5	131
6	Multiscale Modeling of Proteins. <i>Accounts of Chemical Research</i> , 2010, 43, 220-230.	15.6	127
7	Influence of Graphene Curvature on Hydrogen Adsorption: Toward Hydrogen Storage Devices. <i>Journal of Physical Chemistry C</i> , 2013, 117, 11506-11513.	3.1	125
8	A coarse grained model for the dynamics of flap opening in HIV-1 protease. <i>Chemical Physics Letters</i> , 2005, 413, 123-128.	2.6	123
9	Flap opening dynamics in HIV-1 protease explored with a coarse-grained model. <i>Journal of Structural Biology</i> , 2007, 157, 606-615.	2.8	113
10	The Influence of Macromolecular Crowding on HIV-1 Protease Internal Dynamics. <i>Journal of the American Chemical Society</i> , 2006, 128, 6006-6007.	13.7	96
11	Minimalist models for proteins: a comparative analysis. <i>Quarterly Reviews of Biophysics</i> , 2010, 43, 333-371.	5.7	96
12	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.	1.9	87
13	Gated Binding of Ligands to HIV-1 Protease: Brownian Dynamics Simulations in a Coarse-Grained Model. <i>Biophysical Journal</i> , 2006, 90, 3880-3885.	0.5	80
14	Coarse-grained force field for the nucleosome from self-consistent multiscaling. <i>Journal of Computational Chemistry</i> , 2008, 29, 1429-1439.	3.3	77
15	HIV-1 Protease Substrate Binding and Product Release Pathways Explored with Coarse-Grained Molecular Dynamics. <i>Biophysical Journal</i> , 2007, 92, 4179-4187.	0.5	74
16	Graphene-based technologies for energy applications, challenges and perspectives. <i>2D Materials</i> , 2015, 2, 030204.	4.4	74
17	Diffusion within the Cytoplasm: A Mesoscale Model of Interacting Macromolecules. <i>Biophysical Journal</i> , 2014, 107, 2579-2591.	0.5	73
18	GCN5-dependent acetylation of HIV-1 integrase enhances viral integration. <i>Retrovirology</i> , 2010, 7, 18.	2.0	70

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19	Binding Pathways of Ligands to HIV-1 Protease: Coarse-grained and Atomistic Simulations. <i>Chemical Biology and Drug Design</i> , 2007, 69, 5-13.	3.2	67
20	Mapping All-Atom Models onto One-Bead Coarse-Grained Models: A General Properties and Applications to a Minimal Polypeptide Model. <i>Journal of Chemical Theory and Computation</i> , 2006, 2, 667-673.	5.3	64
21	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.	2.6	60
22	Superlubricity of epitaxial monolayer WS ₂ on graphene. <i>Nano Research</i> , 2018, 11, 5946-5956.	10.4	58
23	Photoreversible Dark State in a Tristable Green Fluorescent Protein Variant. <i>Journal of Physical Chemistry B</i> , 2003, 107, 1679-1684.	2.6	57
24	Coherent Dynamics of Photoexcited Green Fluorescent Proteins. <i>Physical Review Letters</i> , 2001, 86, 3439-3442.	7.8	56
25	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, 2366-2377.	3.3	47
26	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, 378-389.	2.6	46
27	Raman Study of Chromophore States in Photochromic Fluorescent Proteins. <i>Journal of the American Chemical Society</i> , 2009, 131, 96-103.	13.7	41
28	Electronic structure and Peierls instability in graphene nanoribbons sculpted in graphene. <i>Physical Review B</i> , 2010, 81, .	3.2	40
29	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.	3.1	39
30	Electronic properties of single-layer tungsten disulfide on epitaxial graphene on silicon carbide. <i>Nanoscale</i> , 2017, 9, 16412-16419.	5.6	39
31	Supercoiling and Local Denaturation of Plasmids with a Minimalist DNA Model. <i>Journal of Physical Chemistry B</i> , 2008, 112, 13197-13200.	2.6	37
32	Fullerene-like III ⁺ V Clusters: A Density Functional Theory Prediction. <i>Journal of Physical Chemistry B</i> , 2001, 105, 12477-12480.	2.6	34
33	Multiscale modeling of proteins interaction with functionalized nanoparticles. <i>Current Opinion in Colloid and Interface Science</i> , 2019, 41, 66-73.	7.4	34
34	Spontaneous Formation and Stability of Small GaP Fullerenes. <i>Physical Review Letters</i> , 2000, 85, 4554-4557.	7.8	31
35	The low frequency vibrational modes of green fluorescent proteins. <i>Chemical Physics</i> , 2003, 287, 33-42.	1.9	31
36	Increasing the active surface of titanium islands on graphene by nitrogen sputtering. <i>Applied Physics Letters</i> , 2015, 106, .	3.3	31

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37	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, 946-958.	2.6	29
38	Evolutionary Algorithm in the Optimization of a Coarse-Grained Force Field. <i>Journal of Chemical Theory and Computation</i> , 2013, 9, 4874-4889.	5.3	28
39	Hydrogen Storage in Rippled Graphene: Perspectives from Multi-Scale Simulations. <i>Frontiers in Materials</i> , 2015, 2, .	2.4	22
40	The Chromophore of asFP595: A Theoretical Study. <i>Journal of Physical Chemistry B</i> , 2006, 110, 9348-9353.	2.6	21
41	Revealing the Multibonding State between Hydrogen and Graphene-Supported Ti Clusters. <i>Journal of Physical Chemistry C</i> , 2016, 120, 12974-12979.	3.1	21
42	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.	1.9	20
43	A Minimalist Model of Protein Diffusion and Interactions: The Green Fluorescent Protein within the Cytoplasm. <i>Macromolecules</i> , 2013, 46, 8311-8322.	4.8	20
44	Intrinsic structural and electronic properties of the Buffer Layer on Silicon Carbide unraveled by Density Functional Theory. <i>Scientific Reports</i> , 2018, 8, 13097.	3.3	20
45	Multistable Rippling of Graphene on SiC: A Density Functional Theory Study. <i>Journal of Physical Chemistry C</i> , 2016, 120, 7670-7677.	3.1	17
46	Engineering 3D Graphene-Based Materials: State of the Art and Perspectives. <i>Molecules</i> , 2020, 25, 339.	3.8	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. <i>Nano Research</i> , 2018, 11, 864-873.	10.4	14
49	A Multi-Scale Multi-Stable Model for the Rhodopsin Photocycle. <i>Molecules</i> , 2014, 19, 14961-14978.	3.8	13
50	From the Buffer Layer to Graphene on Silicon Carbide: Exploring Morphologies by Computer Modeling. <i>Frontiers in Materials</i> , 2019, 6, .	2.4	13
51	Minimalist Model for the Dynamics of Helical Polypeptides: A Statistic-Based Parametrization. <i>Journal of Chemical Theory and Computation</i> , 2014, 10, 3885-3895.	5.3	12
52	Water splitting of hydrogen chemisorbed in graphene oxide dynamically evolves into a graphane lattice. <i>Carbon</i> , 2019, 153, 234-241.	10.3	12
53	Covalent organic functionalization of graphene nanosheets and reduced graphene oxide via 1,3-dipolar cycloaddition of azomethine ylide. <i>Nanoscale Advances</i> , 2021, 3, 5841-5852.	4.6	11
54	Low-Resolution Models for the Interaction Dynamics of Coated Gold Nanoparticles with Î2-microglobulin. <i>International Journal of Molecular Sciences</i> , 2019, 20, 3866.	4.1	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. <i>The Philosophical Magazine: Physics of Condensed Matter B, Statistical Mechanics, Electronic, Optical and Magnetic Properties</i> , 1994, 69, 833-848.	0.6	9
56	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
57	Vibrational Properties of DsRed Model Chromophores. <i>ChemPhysChem</i> , 2005, 6, 1786-1788.	2.1	9
58	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.	1.2	8
59	SecStAnT: secondary structure analysis tool for data selection, statistics and models building. <i>Bioinformatics</i> , 2014, 30, 668-674.	4.1	8
60	Editorial: Multiscale Modeling From Macromolecules to Cell: Opportunities and Challenges of Biomolecular Simulations. <i>Frontiers in Molecular Biosciences</i> , 2020, 7, 194.	3.5	8
61	Unraveling localized states in quasi free standing monolayer graphene by means of Density Functional Theory. <i>Carbon</i> , 2018, 130, 466-474.	10.3	7
62	Vacancy formation energy in the quantal crystals of the two helium isotopes. <i>Philosophical Magazine Letters</i> , 1997, 76, 377-382.	1.2	6
63	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.	1.3	6
64	Structural Transition States Explored With Minimalist Coarse Grained Models: Applications to Calmodulin. <i>Frontiers in Molecular Biosciences</i> , 2019, 6, 104.	3.5	6
65	Vibrational and Elastic Properties of the Wigner Electron Lattice Near Melting. <i>Europhysics Letters</i> , 1993, 23, 433-438.	2.0	5
66	Optimization of Analytical Potentials for Coarse-Grained Biopolymer Models. <i>Journal of Physical Chemistry B</i> , 2016, 120, 8571-8579.	2.6	5
67	Building Minimalist Models for Functionalized Metal Nanoparticles. <i>Frontiers in Molecular Biosciences</i> , 2019, 6, 50.	3.5	5
68	In silico design, building and gas adsorption of nano-porous graphene scaffolds. <i>Nanotechnology</i> , 2021, 32, 045704.	2.6	5
69	Viscoelastic Model for the Transition from Normal to Fast Sound in Water. <i>Physics and Chemistry of Liquids</i> , 1996, 33, 191-198.	1.2	4
70	Lattice vibrations and elastic constants of crystalline and near low-temperature melting. <i>Physica B: Condensed Matter</i> , 1999, 262, 369-380.	2.7	4
71	One-Photon and Two-Photon Excitation of Fluorescent Proteins. <i>Springer Series on Fluorescence</i> , 2011, , 3-40.	0.8	4
72	Hydrogen transport within graphene multilayers by means of flexural phonons. <i>2D Materials</i> , 2015, 2, 014009.	4.4	4

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73	III-V semiconductor nanostructures and iontronics: InAs nanowire-based electric double layer field effect transistors. AIP Conference Proceedings, 2019, , .	0.4	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.	2.7	3
77	Dispersion Laws of Collective Excitations in Crystalline and Superfluid 4 He Related via Density-Functional Theory. Europhysics Letters, 1995, 32, 67-72.	2.0	2
78	SDPhound, a Mutual Information-Based Method to Investigate Specificity-Determining Positions. Algorithms, 2009, 2, 764-789.	2.1	2
79	Collective Mode Mining from Molecular Dynamics Simulations: A Comparative Approach. International Journal of Computational Methods, 2018, 15, 1850108.	1.3	2
80	Evolutionary Switches Structural Transitions via Coarse-Grained Models. Journal of Computational Biology, 2020, 27, 189-199.	1.6	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.	0.7	0
86	GCN5-dependent acetylation of HIV-1 integrase enhances viral integration. Retrovirology, 2009, 6, P20.	2.0	0
87	One-Bead Coarse-Grained Models for Proteins. , 2008, , 285-298.		0