Ana Vila Verde

List of Publications by Year
in descending order

37 papers	816 citations	516710 16 h-index	501196 28 g-index
40 all docs	40 docs citations	40 times ranked	1191 citing authors

#	Article	IF	Citations
1	Investigating the Specificity of Peptide Adsorption on Gold Using Molecular Dynamics Simulations. Biomacromolecules, 2009, 10, 2118-2128.	5.4	121
2	Ultrafast Reorientation of Dangling OH Groups at the Air-Water Interface Using Femtosecond Vibrational Spectroscopy. Physical Review Letters, 2011, 107, 116102.	7.8	84
3	Statics and Dynamics of Free and Hydrogen-Bonded OH Groups at the Air/Water Interface. Journal of Physical Chemistry B, 2012, 116, 9467-9481.	2.6	53
4	Molecular mechanics of coiled coils loaded in the shear geometry. Chemical Science, 2018, 9, 4610-4621.	7.4	48
5	Developing force fields when experimental data is sparse: AMBER/GAFF-compatible parameters for inorganic and alkyl oxoanions. Physical Chemistry Chemical Physics, 2017, 19, 20593-20607.	2.8	45
6	Adsorption of Homopolypeptides on Gold Investigated Using Atomistic Molecular Dynamics. Langmuir, 2011, 27, 5918-5926.	3.5	43
7	Simulation study of micelle formation by bile salts. Soft Matter, 2010, 6, 3815.	2.7	41
8	Temperature-sensitive colloidal phase behavior induced by critical Casimir forces. Journal of Chemical Physics, 2013, 139, 094903.	3.0	41
9	The Multiple Origins of the Hydrophobicity of Fluorinated Apolar Amino Acids. CheM, 2017, 3, 881-897.	11.7	39
10	Disaccharide Topology Induces Slowdown in Local Water Dynamics. Journal of Physical Chemistry B, 2011, 115, 7069-7084.	2.6	37
11	Solvent-shared pairs of densely charged ions induce intense but short-range supra-additive slowdown of water rotation. Physical Chemistry Chemical Physics, 2016, 18, 1918-1930.	2.8	30
12	Unexpected trends in the hydrophobicity of fluorinated amino acids reflect competing changes in polarity and conformation. Physical Chemistry Chemical Physics, 2019, 21, 2029-2038.	2.8	28
13	Cooperative Slowdown of Water Rotation near Densely Charged Ions Is Intense but Short-Ranged. Journal of Physical Chemistry B, 2013, 117, 10556-10566.	2.6	24
14	Hydrophobic but Water-Friendly: Favorable Waterâ€“Perfluoromethyl Interactions Promote Hydration Shell Defects. Journal of the American Chemical Society, 2019, 141, 15856-15868.	13.7	24
15	Influence of Glycosidic Linkage Neighbors on Disaccharide Conformation in Vacuum. Journal of Physical Chemistry B, 2007, 111, 13775-13785.	2.6	19
16	Cooperativity and ion pairing in magnesium sulfate aqueous solutions from the dilute regime to the solubility limit. Physical Chemistry Chemical Physics, 2020, 22, 12140-12153.	2.8	18
17	Is the Solution Activity Derivative Sufficient to Parametrize Ionâ€“Ion Interactions? Ions for TIP5P Water. Journal of Chemical Theory and Computation, 2017, 13, 2112-2122.	5.3	17
18	Benefits in Cost and Reduced Discomfort of New Techniques of Minimally Invasive Cavity Treatment. Journal of Dental Research, 2009, 88, 297-299.	5.2	16

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19	The Free OD at the Air/D₂O Interface Is Structurally and Dynamically Heterogeneous. Journal of Physical Chemistry B, 2013, 117, 11753-11764.	2.6	13
20	Kinetics of formation of bile salt micelles from coarse-grained Langevin dynamics simulations. Soft Matter, 2016, 12, 5172-5179.	2.7	13
21	Trimeric coiled coils expand the range of strength, toughness and dynamics of coiled coil motifs under shear. Physical Chemistry Chemical Physics, 2018, 20, 29105-29115.	2.8	11
22	Unfolding mechanism and free energy landscape of single, stable, alpha helices at low pull speeds. Soft Matter, 2020, 16, 9917-9928.	2.7	6
23	Proteins maintain hydration at high [KCl] concentration regardless of content in acidic amino acids. Biophysical Journal, 2021, 120, 2746-2762.	0.5	6
24	Mesoscopic modelling of the interaction of infrared lasers with composite materials: an application to human dental enamel. Applied Surface Science, 2004, 238, 410-414.	6.1	5
25	Boundary conditions for 3D dynamic models of ablation of ceramics by pulsed mid-infrared lasers. Applied Surface Science, 2005, 247, 354-361.	6.1	5
26	Modelling the influence of pore size on the response of materials to infrared lasers â€“ An application to human enamel. Applied Surface Science, 2005, 248, 446-449.	6.1	4
27	The role of mesoscopic modelling in understanding the response of dental enamel to mid-infrared radiation. Physics in Medicine and Biology, 2007, 52, 2703-2717.	3.0	4
28	Goodness of fit testing in dynamic single-molecule force spectroscopy. Journal of Chemical Physics, 2018, 149, 244120.	3.0	4
29	Quantifying how step-wise fluorination tunes local solute hydrophobicity, hydration shell thermodynamics and the quantum mechanical contributions of soluteâ€“water interactions. Physical Chemistry Chemical Physics, 2020, 22, 22997-23008.	2.8	4
30	Modeling of the human enamel laser ablation process at the mesoscopic scale. , 2003, 4950, 72.		3
31	Mesoscopic modelling of enamel interaction with mid-infrared sub-ablative laser pulses. Thin Solid Films, 2004, 453-454, 89-93.	1.8	3
32	Mechanical and thermal response of enamel to IR radiation: a finite element mesoscopic model. , 2005, , .		2
33	The influence of pulse duration on the stress levels in ablation of ceramics: A finite element study. Applied Surface Science, 2006, 252, 4511-4515.	6.1	2
34	Influence of Methylene Fluorination and Chain Length on the Hydration Shell Structure and Thermodynamics of Linear Diols. Journal of Physical Chemistry B, 2021, 125, 13552-13564.	2.6	1
35	Comment on â€œPrincipal Role of the Stepwise Aggregation Mechanism in Ionic Surfactant Solutions Near the Critical Micelle Concentration. Molecular Dynamics Studyâ€• Journal of Physical Chemistry B, 2011, 115, 1927-1927.	2.6	0
36	How Biomolecules Influence Water Structure and Dynamics. Biophysical Journal, 2011, 100, 195a.	0.5	0

#	Article	IF	Citations
37	Tribute to Dor Ben-Amotz. Journal of Physical Chemistry B, 2022, 126, 2943-2945.	2.6	0