

Lucio Colombi Ciacchi

List of Publications by Year in descending order

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103
papers

3,681
citations

126708

33
h-index

143772

57
g-index

107
all docs

107
docs citations

107
times ranked

4880
citing authors

#	ARTICLE	IF	CITATIONS
1	A review of contact force models between nanoparticles in agglomerates, aggregates, and films. <i>Journal of Aerosol Science</i> , 2021, 153, 105719.	1.8	61
2	Lessons from a Challenging System: Accurate Adsorption Free Energies at the Amino Acid/ZnO Interface. <i>Journal of Chemical Theory and Computation</i> , 2021, 17, 4420-4434.	2.3	5
3	Water Reactions on Reconstructed Rutile TiO ₂ : A Density Functional Theory/Density Functional Tight Binding Approach. <i>Journal of Physical Chemistry C</i> , 2021, 125, 13234-13246.	1.5	9
4	Mathematical aspects of catalyst positioning in lithium/air batteries. <i>Inverse Problems</i> , 2020, 36, 044001.	1.0	0
5	Strong Macroscale Supercrystalline Structures by 3D Printing Combined with Self-Assembly of Ceramic Functionalized Nanoparticles. <i>Advanced Engineering Materials</i> , 2020, 22, 2070028.	1.6	2
6	Strong Macroscale Supercrystalline Structures by 3D Printing Combined with Self-Assembly of Ceramic Functionalized Nanoparticles. <i>Advanced Engineering Materials</i> , 2020, 22, 2000352.	1.6	19
7	A Contact Model for the Discrete Element Simulations of Aggregated Nanoparticle Films. , 2019, , 339-358.		0
8	Impact of the Conformational Variability of Oligopeptides on the Computational Prediction of Their CD Spectra. <i>Journal of Physical Chemistry B</i> , 2019, 123, 6694-6704.	1.2	7
9	Platform for Screening Abiotic/Biotic Interactions Using Indicator Displacement Assays. <i>Langmuir</i> , 2019, 35, 14230-14237.	1.6	3
10	Bio-interfactants as double-sided tapes for graphene oxide. <i>Nanoscale</i> , 2019, 11, 4236-4247.	2.8	5
11	Force spectroscopic detection of peptide cleavage by thrombin exploiting biotin-streptavidin interactions in a bio-sensing context. <i>Analytical Methods</i> , 2019, 11, 1102-1110.	1.3	5
12	Mineralization of iron oxide by ferritin homopolymers immobilized on SiO ₂ nanoparticles. <i>Bioinspired, Biomimetic and Nanobiomaterials</i> , 2019, 8, 16-27.	0.7	1
13	Compaction-induced restructuring of aggregated nanoparticle films using the discrete element method. <i>Powder Technology</i> , 2019, 342, 773-779.	2.1	15
14	Anti-Staphylococcal Calopins from Fruiting Bodies of <i>Caloboletus radicans</i> . <i>Journal of Natural Products</i> , 2018, 81, 400-404.	1.5	6
15	Anchoring of Iron Oxyhydroxide Clusters at H and L Ferritin Subunits. <i>ACS Biomaterials Science and Engineering</i> , 2018, 4, 483-490.	2.6	5
16	Ligand-functionalized Pt nanoparticles as asymmetric heterogeneous catalysts: molecular reaction control by ligand-reactant interactions. <i>Catalysis Science and Technology</i> , 2018, 8, 6062-6075.	2.1	19
17	Atomistic Details of Chymotrypsin Conformational Changes upon Adsorption on Silica. <i>ACS Biomaterials Science and Engineering</i> , 2018, 4, 4036-4050.	2.6	15
18	Structural and Computational Assessment of the Influence of Wet-Chemical Post-Processing of the Al-Substituted Cubic Li ₇ La ₃ Zr ₂ O ₁₂ . <i>ACS Applied Materials & Interfaces</i> , 2018, 10, 37188-37197.	4.0	30

#	ARTICLE	IF	CITATIONS
19	Graphene-based nanoplatfoms for surface-enhanced Raman scattering sensing. <i>Analyst</i> , The, 2018, 143, 5074-5089.	1.7	50
20	Atomistic Modeling of the Formation of a Thermoset/Thermoplastic Interphase during Co-Curing. <i>Macromolecules</i> , 2018, 51, 3983-3993.	2.2	35
21	Interactions at the Silica-Peptide Interface: Influence of the Extent of Functionalization on the Conformational Ensemble. <i>Langmuir</i> , 2018, 34, 8255-8263.	1.6	18
22	Recent Advances in Nanoporous Membranes for Water Purification. <i>Nanomaterials</i> , 2018, 8, 65.	1.9	136
23	Simulated and experimental force spectroscopy of lysozyme on silica. <i>Physical Chemistry Chemical Physics</i> , 2018, 20, 19595-19605.	1.3	11
24	A new contact model for the discrete element method simulation of TiO_2 nanoparticle films under mechanical load. <i>Granular Matter</i> , 2018, 20, 1.	1.1	11
25	Molecular Dynamics Simulations of the Silica-Cell Membrane Interaction: Insights on Biomineralization and Nanotoxicity. <i>Journal of Physical Chemistry C</i> , 2018, 122, 21330-21343.	1.5	23
26	Variability of Zinc Oxide Dissolution Rates. <i>Environmental Science & Technology</i> , 2017, 51, 4297-4305.	4.6	37
27	Adsorption of DNA Fragments at Aqueous Graphite and Au(111) via Integration of Experiment and Simulation. <i>Langmuir</i> , 2017, 33, 10193-10204.	1.6	22
28	Creation of models and parametrization of a classical force field for amorphous Al_2O_3 /water interfaces based on Density Functional Theory. <i>Computational Materials Science</i> , 2017, 140, 307-314.	1.4	10
29	Dependencies of the Adhesion Forces between TiO_2 Nanoparticles on Size and Ambient Humidity. <i>Journal of Physical Chemistry C</i> , 2017, 121, 15294-15303.	1.5	17
30	Growth and structure of ultrathin praseodymium oxide layers on ruthenium(0001). <i>Physical Chemistry Chemical Physics</i> , 2017, 19, 3480-3485.	1.3	12
31	Irreversible Damage of Polymer Membranes During Attenuated Total Reflection Infrared Analysis. <i>Applied Spectroscopy</i> , 2017, 71, 1127-1133.	1.2	7
32	Recent Advances in the Synthesis of Graphene-Based Nanomaterials for Controlled Drug Delivery. <i>Applied Sciences (Switzerland)</i> , 2017, 7, 1175.	1.3	63
33	Physisorption of β -chymotrypsin on SiO_2 and TiO_2 : A comparative study via experiments and molecular dynamics simulations. <i>Biointerphases</i> , 2016, 11, 011007.	0.6	12
34	Ultrasooth $\text{Ru}(0001)$ Films as Templates for Ceria Nanoarchitectures. <i>Crystal Growth and Design</i> , 2016, 16, 4216-4224.	1.4	15
35	Contact mechanics of highly porous oxide nanoparticle agglomerates. <i>Journal of Nanoparticle Research</i> , 2016, 18, 200.	0.8	26
36	AFM-based force spectroscopy for bioimaging and biosensing. <i>RSC Advances</i> , 2016, 6, 12893-12912.	1.7	56

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37	Nanoscale Properties of Solid-Liquid Interfaces. , 2016, , 2692-2698.		0
38	Assessment of the Proteolytic Activity of $\hat{\pm}$ -Chymotrypsin Immobilized on Colloidal Particles by Matrix-Assisted Laser Desorption Ionization Time-of-Flight Mass Spectrometry. Analytical Letters, 2015, 48, 424-441.	1.0	6
39	Accuracy of buffered-force QM/MM simulations of silica. Journal of Chemical Physics, 2015, 142, 064116.	1.2	17
40	Dental implants coated with a durable and antibacterial film. Surface Innovations, 2015, 3, 27-38.	1.4	18
41	A novel aptasensor based on single-molecule force spectroscopy for highly sensitive detection of mercury ions. Analyst, The, 2015, 140, 5243-5250.	1.7	29
42	Physisorption of enzymatically active chymotrypsin on titania colloidal particles. Journal of Colloid and Interface Science, 2015, 455, 236-244.	5.0	13
43	Estimation of the free energy of adsorption of a polypeptide on amorphous SiO_2 from molecular dynamics simulations and force spectroscopy experiments. Soft Matter, 2015, 11, 6254-6265.	1.2	30
44	In situ high temperature X-ray diffraction, transmission electron microscopy and theoretical modeling for the formation of WO_3 crystallites. CrystEngComm, 2015, 17, 6985-6998.	1.3	46
45	Label-Free Sensing of Adenosine Based on Force Variations Induced by Molecular Recognition. Biosensors, 2015, 5, 85-97.	2.3	13
46	Gas-solid catalytic reactions with an extended DSMC model. AIChE Journal, 2015, 61, 2092-2103.	1.8	11
47	Adsorption Orientation and Binding Motifs of Lysozyme and Chymotrypsin on Amorphous Silica. Journal of Physical Chemistry C, 2015, 119, 7295-7307.	1.5	43
48	Contact Forces between TiO_2 Nanoparticles Governed by an Interplay of Adsorbed Water Layers and Roughness. Langmuir, 2015, 31, 11288-11295.	1.6	40
49	Atomistic Modeling of the Charge Process in Lithium/Air Batteries. Journal of Physical Chemistry C, 2015, 119, 25807-25817.	1.5	8
50	Optimization of Catalytically Active Sites Positioning in Porous Cathodes of Lithium/Air Batteries Filled with Different Electrolytes. Journal of the Electrochemical Society, 2015, 162, A2796-A2804.	1.3	16
51	Selective covalent immobilization of ferritin on alumina. Biointerphases, 2014, 9, 031018.	0.6	9
52	Direct force measurements on peeling heteropolymer ssDNA from a graphite surface using single-molecule force spectroscopy. Physical Chemistry Chemical Physics, 2014, 16, 3995.	1.3	23
53	Identification of materials' binding peptide sequences guided by a MALDI-ToF MS depletion assay. Analytical Methods, 2014, 6, 1501-1509.	1.3	5
54	Parametrization of a classical force field for iron oxyhydroxide/water interfaces based on Density Functional Theory calculations. Computational Materials Science, 2014, 92, 343-352.	1.4	15

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55	Molecular dynamics simulations of the amino acid-ZnO (10-10) interface: A comparison between density functional theory and density functional tight binding results. <i>Journal of Chemical Physics</i> , 2014, 140, 234707.	1.2	11
56	Computational Prediction of Circular Dichroism Spectra and Quantification of Helicity Loss upon Peptide Adsorption on Silica. <i>Langmuir</i> , 2014, 30, 3487-3494.	1.6	35
57	DFT study of reaction processes of methane combustion on PdO(100). <i>Chemical Physics</i> , 2014, 443, 53-60.	0.9	25
58	Molecular dynamics simulations on scattering of single Ar, N ₂ , and CO ₂ molecules on realistic surfaces. <i>Computers and Fluids</i> , 2014, 97, 31-39.	1.3	26
59	Computational prediction of heterogeneous interface properties at the atomic level. <i>Journal of Cheminformatics</i> , 2013, 5, .	2.8	1
60	Label-free biosensing with single-molecule force spectroscopy. <i>Chemical Communications</i> , 2013, 49, 3239.	2.2	19
61	Label-free molecular detection with capped carbon nanotubes. <i>Applied Physics Letters</i> , 2013, 102, 083103.	1.5	1
62	Atomistic Simulations of the ZnO(11̄0)/Water Interface: A Comparison between First-Principles, Tight-Binding, and Empirical Methods. <i>Journal of Chemical Theory and Computation</i> , 2012, 8, 4517-4526.	2.3	21
63	Specific Material Recognition by Small Peptides Mediated by the Interfacial Solvent Structure. <i>Journal of the American Chemical Society</i> , 2012, 134, 2407-2413.	6.6	131
64	Adhesion Mechanisms of the Contact Interface of TiO ₂ Nanoparticles in Films and Aggregates. <i>Langmuir</i> , 2012, 28, 11457-11464.	1.6	71
65	<i>Ab initio</i> derived force field parameters for molecular dynamics simulations of deprotonated amorphous SiO ₂ /water interfaces. <i>Physica Status Solidi (B): Basic Research</i> , 2012, 249, 292-305.	0.7	71
66	Back Cover: <i>Ab initio</i> derived force field parameters for molecular dynamics simulations of deprotonated amorphous SiO ₂ /water interfaces (Phys. Status Solidi B 2(2012)). <i>Physica Status Solidi (B): Basic Research</i> , 2012, 249, .	0.7	1
67	A Classical Potential to Model the Adsorption of Biological Molecules on Oxidized Titanium Surfaces. <i>Journal of Chemical Theory and Computation</i> , 2011, 7, 473-484.	2.3	54
68	Adsorption and Reduction of Glutathione Disulfide on γ -Al ₂ O ₃ Nanoparticles: Experiments and Modeling. <i>Langmuir</i> , 2011, 27, 9449-9457.	1.6	18
69	Electronic Transport in Natively Oxidized Silicon Nanowires. <i>ACS Nano</i> , 2011, 5, 2839-2846.	7.3	11
70	First principles and classical modeling of the oxidized titanium (0001) surface. <i>Surface Science</i> , 2010, 604, 1105-1115.	0.8	38
71	Atomically Smooth Stress-Corrosion Cleavage of a Hydrogen-Implanted Crystal. <i>Physical Review Letters</i> , 2010, 105, 075502.	2.9	29
72	Origin of the Selective Cr Oxidation in CoCr Alloy Surfaces. <i>Journal of Physical Chemistry Letters</i> , 2010, 1, 2343-2348.	2.1	15

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73	Mechanisms of Initial Oxidation of the Co(0001) and Cr(110) Surfaces. <i>Journal of Physical Chemistry C</i> , 2010, 114, 6614-6623.	1.5	20
74	Vacancy segregation in the initial oxidation stages of the TiN(100) surface. <i>Journal of Chemical Physics</i> , 2009, 130, 134714.	1.2	38
75	Multiscale mechanics modeling of direct silicon wafer bonding. <i>Scripta Materialia</i> , 2009, 60, 1125-1128.	2.6	9
76	Atomic-Level Studies of Molecular Self-Assembly on Metallic Surfaces. <i>Advanced Materials</i> , 2009, 21, 1055-1066.	11.1	17
77	Dissociative Adsorption of Methane on Surface Oxide Structures of Pd~Pt Alloys. <i>Journal of Physical Chemistry C</i> , 2009, 113, 21097-21105.	1.5	18
78	Density functional theory study of Fe(II) adsorption and oxidation on goethite surfaces. <i>Physical Review B</i> , 2009, 79, .	1.1	59
79	Water structuring and collagen adsorption at hydrophilic and hydrophobic silicon surfaces. <i>Physical Chemistry Chemical Physics</i> , 2009, 11, 11395.	1.3	50
80	DFT modelling of ceramic materials and interfaces. <i>International Journal of Materials and Product Technology</i> , 2009, 35, 271.	0.1	0
81	Ab initio study of element segregation and oxygen adsorption on PtPd and CoCr binary alloy surfaces. <i>Surface Science</i> , 2008, 602, 876-884.	0.8	31
82	Stress-Driven Oxidation Chemistry of Wet Silicon Surfaces. <i>Journal of Physical Chemistry C</i> , 2008, 112, 12077-12080.	1.5	30
83	DFT Study of the Thermodynamic Stability of Pd~Pt Bulk Oxide Phases. <i>Journal of Physical Chemistry C</i> , 2008, 112, 13623-13628.	1.5	28
84	DFT Modelling of Oxygen Adsorption on CoCr Surfaces. , 2008, , 173-186.		0
85	Development of a classical force field for the oxidized Si surface: Application to hydrophilic wafer bonding. <i>Journal of Chemical Physics</i> , 2007, 127, 204704.	1.2	68
86	Modelling the onset of oxide formation on metal surfaces from first principles. <i>International Journal of Materials Research</i> , 2007, 98, 708-716.	0.1	17
87	Structure and Energetics of Diphenylalanine Self-Assembling on Cu(110). <i>Journal of Physical Chemistry A</i> , 2007, 111, 12740-12748.	1.1	34
88	Tracking the Chiral Recognition of Adsorbed Dipeptides at the Single-Molecule Level. <i>Angewandte Chemie - International Edition</i> , 2007, 46, 4492-4495.	7.2	148
89	Stress development and impurity segregation during oxidation of the Si(100) surface. <i>Surface Science</i> , 2007, 601, 4888-4898.	0.8	9
90	Modelling (100) hydrogen-induced platelets in silicon with a multi-scale molecular dynamics approach. <i>Physica B: Condensed Matter</i> , 2007, 401-402, 16-20.	1.3	3

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91	Density functional theory study of platinum oxides: From infinite crystals to nanoscopic particles. <i>Physical Review B</i> , 2007, 76, .	1.1	77
92	Catalytic Oxidation Activity of Pt ₃ O ₄ Surfaces and Thin Films. <i>Journal of Physical Chemistry B</i> , 2006, 110, 14860-14869.	1.2	133
93	Novel Structural Features of CDK Inhibition Revealed by an ab Initio Computational Method Combined with Dynamic Simulations. <i>Journal of Medicinal Chemistry</i> , 2006, 49, 5141-5153.	2.9	37
94	First-Principles Molecular-Dynamics Study of Native Oxide Growth on Si(001). <i>Physical Review Letters</i> , 2005, 95, 196101.	2.9	67
95	Hot-Atom O ₂ Dissociation and Oxide Nucleation on Al(111). <i>Physical Review Letters</i> , 2004, 92, 176104.	2.9	76
96	Bioactivity of TiN-coated titanium implants. <i>Acta Materialia</i> , 2004, 52, 1237-1245.	3.8	220
97	Synthesis of Platinum Cluster Chains on DNA Templates: Conditions for a Template-Controlled Cluster Growth. <i>Journal of Physical Chemistry B</i> , 2004, 108, 10801-10811.	1.2	173
98	The entry pathway of O ₂ into human ferritin. <i>Chemical Physics Letters</i> , 2004, 390, 491-495.	1.2	12
99	Growth of Platinum Clusters via Addition of Pt(II) Complexes: A First Principles Investigation. <i>Journal of Physical Chemistry B</i> , 2003, 107, 1755-1764.	1.2	76
100	Nucleation of platinum clusters on biopolymers: a first principles study of the molecular mechanisms. <i>Nanotechnology</i> , 2003, 14, 840-848.	1.3	36
101	DNA as a Selective Metallization Template. <i>Nano Letters</i> , 2002, 2, 841-844.	4.5	304
102	Initial Nucleation of Platinum Clusters after Reduction of K ₂ PtCl ₄ in Aqueous Solution: A First Principles Study. <i>Journal of the American Chemical Society</i> , 2001, 123, 7371-7380.	6.6	114
103	Deposition of calcium ions on rutile (110): a first-principles investigation. <i>Acta Materialia</i> , 2001, 49, 2169-2177.	3.8	86