Lucio Colombi Ciacchi

List of Publications by Year
in descending order

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	DNA as a Selective Metallization Template. Nano Letters, 2002, 2, 841-844.	4.5	304
2	Bioactivity of TiN-coated titanium implants. Acta Materialia, 2004, 52, 1237-1245.	3.8	220
3	Synthesis of Platinum Cluster Chains on DNA Templates:Â Conditions for a Template-Controlled Cluster Growth. Journal of Physical Chemistry B, 2004, 108, 10801-10811.	1.2	173
4	Tracking the Chiral Recognition of Adsorbed Dipeptides at the Single-Molecule Level. Angewandte Chemie - International Edition, 2007, 46, 4492-4495.	7.2	148
5	Recent Advances in Nanoporous Membranes for Water Purification. Nanomaterials, 2018, 8, 65.	1.9	136
6	Catalytic Oxidation Activity of Pt3O4Surfaces and Thin Films. Journal of Physical Chemistry B, 2006, 110, 14860-14869.	1.2	133
7	Specific Material Recognition by Small Peptides Mediated by the Interfacial Solvent Structure. Journal of the American Chemical Society, 2012, 134, 2407-2413.	6.6	131
8	Initial Nucleation of Platinum Clusters after Reduction of K2PtCl4in Aqueous Solution:Â A First Principles Study. Journal of the American Chemical Society, 2001, 123, 7371-7380.	6.6	114
9	Deposition of calcium ions on rutile (110): a first-principles investigation. Acta Materialia, 2001, 49, 2169-2177.	3.8	86
10	Density functional theory study of platinum oxides: From infinite crystals to nanoscopic particles. Physical Review B, 2007, 76, .	1.1	77
11	Growth of Platinum Clusters via Addition of Pt(II) Complexes:Â A First Principles Investigation. Journal of Physical Chemistry B, 2003, 107, 1755-1764.	1.2	76
12	â€œHot-Atomâ€O2Dissociation and Oxide Nucleation on Al(111). Physical Review Letters, 2004, 92, 176104.	2.9	76
13	Adhesion Mechanisms of the Contact Interface of TiO₂ Nanoparticles in Films and Aggregates. Langmuir, 2012, 28, 11457-11464.	1.6	71
14	Ab initio derived forceâ€field parameters for molecular dynamics simulations of deprotonated amorphousâ€SiO₂/water interfaces. Physica Status Solidi (B): Basic Research, 2012, 249, 292-305.	0.7	71
15	Development of a classical force field for the oxidized Si surface: Application to hydrophilic wafer bonding. Journal of Chemical Physics, 2007, 127, 204704.	1.2	68
16	First-Principles Molecular-Dynamics Study of Native Oxide Growth on Si(001). Physical Review Letters, 2005, 95, 196101.	2.9	67
17	Recent Advances in the Synthesis of Graphene-Based Nanomaterials for Controlled Drug Delivery. Applied Sciences (Switzerland), 2017, 7, 1175.	1.3	63
18	A review of contact force models between nanoparticles in agglomerates, aggregates, and films. Journal of Aerosol Science, 2021, 153, 105719.	1.8	61

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19	Density functional theory study of Fe(II) adsorption and oxidation on goethite surfaces. Physical Review B, 2009, 79, .	1.1	59
20	AFM-based force spectroscopy for bioimaging and biosensing. RSC Advances, 2016, 6, 12893-12912.	1.7	56
21	A Classical Potential to Model the Adsorption of Biological Molecules on Oxidized Titanium Surfaces. Journal of Chemical Theory and Computation, 2011, 7, 473-484.	2.3	54
22	Water structuring and collagen adsorption at hydrophilic and hydrophobic silicon surfaces. Physical Chemistry Chemical Physics, 2009, 11, 11395.	1.3	50
23	Graphene-based nanoplatforms for surface-enhanced Raman scattering sensing. Analyst, The, 2018, 143, 5074-5089.	1.7	50
24	In situ high temperature X-ray diffraction, transmission electron microscopy and theoretical modeling for the formation of WO₃ crystallites. CrystEngComm, 2015, 17, 6985-6998.	1.3	46
25	Adsorption Orientation and Binding Motifs of Lysozyme and Chymotrypsin on Amorphous Silica. Journal of Physical Chemistry C, 2015, 119, 7295-7307.	1.5	43
26	Contact Forces between TiO2Nanoparticles Governed by an Interplay of Adsorbed Water Layers and Roughness. Langmuir, 2015, 31, 11288-11295.	1.6	40
27	Vacancy segregation in the initial oxidation stages of the TiN(100) surface. Journal of Chemical Physics, 2009, 130, 134714.	1.2	38
28	First principles and classical modeling of the oxidized titanium (0001) surface. Surface Science, 2010, 604, 1105-1115.	0.8	38
29	Novel Structural Features of CDK Inhibition Revealed by an ab Initio Computational Method Combined with Dynamic Simulations. Journal of Medicinal Chemistry, 2006, 49, 5141-5153.	2.9	37
30	Variability of Zinc Oxide Dissolution Rates. Environmental Science & Technology, 2017, 51, 4297-4305.	4.6	37
31	Nucleation of platinum clusters on biopolymers: a first principles study of the molecular mechanisms. Nanotechnology, 2003, 14, 840-848.	1.3	36
32	Computational Prediction of Circular Dichroism Spectra and Quantification of Helicity Loss upon Peptide Adsorption on Silica. Langmuir, 2014, 30, 3487-3494.	1.6	35
33	Atomistic Modeling of the Formation of a Thermoset/Thermoplastic Interphase during Co-Curing. Macromolecules, 2018, 51, 3983-3993.	2.2	35
34	Structure and Energetics of Diphenylalanine Self-Assembling on Cu(110). Journal of Physical Chemistry A, 2007, 111, 12740-12748.	1.1	34
35	Ab initio study of element segregation and oxygen adsorption on PtPd and CoCr binary alloy surfaces. Surface Science, 2008, 602, 876-884.	0.8	31
36	Stress-Driven Oxidation Chemistry of Wet Silicon Surfaces. Journal of Physical Chemistry C, 2008, 112, 12077-12080.	1.5	30

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37	Estimation of the free energy of adsorption of a polypeptide on amorphous SiO₂ from molecular dynamics simulations and force spectroscopy experiments. Soft Matter, 2015, 11, 6254-6265.	1.2	30
38	Structural and Computational Assessment of the Influence of Wet-Chemical Post-Processing of the Al-Substituted Cubic Li₇La₃Zr₂O₁₂. ACS Applied Materials & Interfaces, 2018, 10, 37188-37197.	4.0	30
39	Atomically Smooth Stress-Corrosion Cleavage of a Hydrogen-Implanted Crystal. Physical Review Letters, 2010, 105, 075502.	2.9	29
40	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
41	DFT Study of the Thermodynamic Stability of Pdâ^'Pt Bulk Oxide Phases. Journal of Physical Chemistry C, 2008, 112, 13623-13628.	1.5	28
42	Molecular dynamics simulations on scattering of single Ar, N2, and CO2 molecules on realistic surfaces. Computers and Fluids, 2014, 97, 31-39.	1.3	26
43	Contact mechanics of highly porous oxide nanoparticle agglomerates. Journal of Nanoparticle Research, 2016, 18, 200.	0.8	26
44	DFT study of reaction processes of methane combustion on PdO(100). Chemical Physics, 2014, 443, 53-60.	0.9	25
45	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
46	Molecular Dynamics Simulations of the Silicaâ€“Cell Membrane Interaction: Insights on Biomineralization and Nanotoxicity. Journal of Physical Chemistry C, 2018, 122, 21330-21343.	1.5	23
47	Adsorption of DNA Fragments at Aqueous Graphite and Au(111) via Integration of Experiment and Simulation. Langmuir, 2017, 33, 10193-10204.	1.6	22
48	Atomistic Simulations of the ZnO(12Ì…10)/Water Interface: A Comparison between First-Principles, Tight-Binding, and Empirical Methods. Journal of Chemical Theory and Computation, 2012, 8, 4517-4526.	2.3	21
49	Mechanisms of Initial Oxidation of the Co(0001) and Cr(110) Surfaces. Journal of Physical Chemistry C, 2010, 114, 6614-6623.	1.5	20
50	Label-free biosensing with single-molecule force spectroscopy. Chemical Communications, 2013, 49, 3239.	2.2	19
51	Ligand-functionalized Pt nanoparticles as asymmetric heterogeneous catalysts: molecular reaction control by ligandâ€“reactant interactions. Catalysis Science and Technology, 2018, 8, 6062-6075.	2.1	19
52	Strong Macroscale Supercrystalline Structures by 3D Printing Combined with Selfâ€Assembly of Ceramic Functionalized Nanoparticles. Advanced Engineering Materials, 2020, 22, 2000352.	1.6	19
53	Dissociative Adsorption of Methane on Surface Oxide Structures of Pdâ^'Pt Alloys. Journal of Physical Chemistry C, 2009, 113, 21097-21105.	1.5	18
54	Adsorption and Reduction of Glutathione Disulfide on Î±-Al2O3Nanoparticles: Experiments and Modeling. Langmuir, 2011, 27, 9449-9457.	1.6	18

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55	Dental implants coated with a durable and antibacterial film. Surface Innovations, 2015, 3, 27-38.	1.4	18
56	Interactions at the Silicaâ€“Peptide Interface: Influence of the Extent of Functionalization on the Conformational Ensemble. Langmuir, 2018, 34, 8255-8263.	1.6	18
57	Modelling the onset of oxide formation on metal surfaces from first principles. International Journal of Materials Research, 2007, 98, 708-716.	0.1	17
58	Atomicâ€Level Studies of Molecular Selfâ€Assembly on Metallic Surfaces. Advanced Materials, 2009, 21, 1055-1066.	11.1	17
59	Accuracy of buffered-force QM/MM simulations of silica. Journal of Chemical Physics, 2015, 142, 064116.	1.2	17
60	Dependencies of the Adhesion Forces between TiO₂ Nanoparticles on Size and Ambient Humidity. Journal of Physical Chemistry C, 2017, 121, 15294-15303.	1.5	17
61	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
62	Origin of the Selective Cr Oxidation in CoCr Alloy Surfaces. Journal of Physical Chemistry Letters, 2010, 1, 2343-2348.	2.1	15
63	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
64	Ultrasmooth Ru(0001) Films as Templates for Ceria Nanoarchitectures. Crystal Growth and Design, 2016, 16, 4216-4224.	1.4	15
65	Atomistic Details of Chymotrypsin Conformational Changes upon Adsorption on Silica. ACS Biomaterials Science and Engineering, 2018, 4, 4036-4050.	2.6	15
66	Compaction-induced restructuring of aggregated nanoparticle films using the discrete element method. Powder Technology, 2019, 342, 773-779.	2.1	15
67	Physisorption of enzymatically active chymotrypsin on titania colloidal particles. Journal of Colloid and Interface Science, 2015, 455, 236-244.	5.0	13
68	Label-Free Sensing of Adenosine Based on Force Variations Induced by Molecular Recognition. Biosensors, 2015, 5, 85-97.	2.3	13
69	The entry pathway of O2 into human ferritin. Chemical Physics Letters, 2004, 390, 491-495.	1.2	12
70	Physisorption of Î±-chymotrypsin on SiO2 and TiO2: A comparative study via experiments and molecular dynamics simulations. Biointerphases, 2016, 11, 011007.	0.6	12
71	Growth and structure of ultrathin praseodymium oxide layers on ruthenium(0001). Physical Chemistry Chemical Physics, 2017, 19, 3480-3485.	1.3	12
72	Electronic Transport in Natively Oxidized Silicon Nanowires. ACS Nano, 2011, 5, 2839-2846.	7.3	11

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73	Molecular dynamics simulations of the amino acid-ZnO (10-10) interface: A comparison between density functional theory and density functional tight binding results. Journal of Chemical Physics, 2014, 140, 234707.	1.2	11
74	Gasâ€solid catalytic reactions with an extended <scp>DSMC</scp> model. AICHE Journal, 2015, 61, 2092-2103.	1.8	11
75	Simulated and experimental force spectroscopy of lysozyme on silica. Physical Chemistry Chemical Physics, 2018, 20, 19595-19605.	1.3	11
76	A new contact model for the discrete element method simulation of $$hbox {TiO}_2$$ TiO 2 nanoparticle films under mechanical load. Granular Matter, 2018, 20, 1.	1.1	11
77	Creation of models and parametrization of a classical force field for amorphous Al2O3/water interfaces based on Density Functional Theory. Computational Materials Science, 2017, 140, 307-314.	1.4	10
78	Stress development and impurity segregation during oxidation of the Si(100) surface. Surface Science, 2007, 601, 4888-4898.	0.8	9
79	Multiscale mechanics modeling of direct silicon wafer bonding. Scripta Materialia, 2009, 60, 1125-1128.	2.6	9
80	Selective covalent immobilization of ferritin on alumina. Biointerphases, 2014, 9, 031018.	0.6	9
81	Water Reactions on Reconstructed Rutile TiO₂: A Density Functional Theory/Density Functional Tight Binding Approach. Journal of Physical Chemistry C, 2021, 125, 13234-13246.	1.5	9
82	Atomistic Modeling of the Charge Process in Lithium/Air Batteries. Journal of Physical Chemistry C, 2015, 119, 25807-25817.	1.5	8
83	Irreversible Damage of Polymer Membranes During Attenuated Total Reflection Infrared Analysis. Applied Spectroscopy, 2017, 71, 1127-1133.	1.2	7
84	Impact of the Conformational Variability of Oligopeptides on the Computational Prediction of Their CD Spectra. Journal of Physical Chemistry B, 2019, 123, 6694-6704.	1.2	7
85	Assessment of the Proteolytic Activity of Î±-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
86	Anti-Staphylococcal Calopins from Fruiting Bodies of Caloboletus radicans. Journal of Natural Products, 2018, 81, 400-404.	1.5	6
87	Identification of materials' binding peptide sequences guided by a MALDI-ToF MS depletion assay. Analytical Methods, 2014, 6, 1501-1509.	1.3	5
88	Anchoring of Iron Oxyhydroxide Clusters at H and L Ferritin Subunits. ACS Biomaterials Science and Engineering, 2018, 4, 483-490.	2.6	5
89	Bio-interfactants as double-sided tapes for graphene oxide. Nanoscale, 2019, 11, 4236-4247.	2.8	5
90	Force spectroscopic detection of peptide cleavage by thrombin exploiting biotinâ€“streptavidin interactions in a bio-sensing context. Analytical Methods, 2019, 11, 1102-1110.	1.3	5

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91	Lessons from a Challenging System: Accurate Adsorption Free Energies at the Amino Acid/ZnO Interface. Journal of Chemical Theory and Computation, 2021, 17, 4420-4434.	2.3	5
92	Modelling (100) hydrogen-induced platelets in silicon with a multi-scale molecular dynamics approach. Physica B: Condensed Matter, 2007, 401-402, 16-20.	1.3	3
93	Platform for Screening Abiotic/Biotic Interactions Using Indicator Displacement Assays. Langmuir, 2019, 35, 14230-14237.	1.6	3
94	Strong Macroscale Supercrystalline Structures by 3D Printing Combined with Selfâ€Assembly of Ceramic Functionalized Nanoparticles. Advanced Engineering Materials, 2020, 22, 2070028.	1.6	2
95	Back Cover: Ab initio derived forceâ€field parameters for molecular dynamics simulations of deprotonated amorphousâ€SiO₂/water interfaces (Phys. Status Solidi B 2/2012). Physica Status Solidi (B): Basic Research, 2012, 249, .	0.7	1
96	Computational prediction of heterogeneous interface properties at the atomic level. Journal of Cheminformatics, 2013, 5, .	2.8	1
97	Label-free molecular detection with capped carbon nanotubes. Applied Physics Letters, 2013, 102, 083103.	1.5	1
98	Mineralization of iron oxide by ferritin homopolymers immobilized on SiO₂ nanoparticles. Bioinspired, Biomimetic and Nanobiomaterials, 2019, 8, 16-27.	0.7	1
99	DFT modelling of ceramic materials and interfaces. International Journal of Materials and Product Technology, 2009, 35, 271.	0.1	0
100	A Contact Model for the Discrete Element Simulations of Aggregated Nanoparticle Films. , 2019, , 339-358.		0
101	Mathematical aspects of catalyst positioning in lithium/air batteries. Inverse Problems, 2020, 36, 044001.	1.0	0
102	Nanoscale Properties of Solidâ€“Liquid Interfaces. , 2016, , 2692-2698.		0
103	DFT Modelling of Oxygen Adsorption on CoCr Surfaces. , 2008, , 173-186.		0