Massimo Celino

List of Publications by Year
in descending order

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75 papers	1,593 citations	430754 18 h-index	302012 39 g-index
77 all docs	77 docs citations	77 times ranked	1892 citing authors

#	Article	IF	Citations
1	Ab Initio Study of Octane Moiety Adsorption on H- and Cl-Functionalized Silicon Nanowires. Nanomaterials, 2022, 12, 1590.	1.9	2
2	Enhancing the electronic properties of VLS-grown silicon nanowires by surface charge transfer. Applied Surface Science, 2022, 599, 153957.	3.1	4
3	Theoretical and Computational Study of the Sphere-to-Rod Transition of Triton X-100 Micellar Nanoscale Aggregates in Aqueous Solution: Implications for Membrane Protein Purification and Membrane Solubilization. ACS Applied Nano Materials, 2021, 4, 4552-4561.	2.4	11
4	Tuning the Electronic Properties of Graphane via Hydroxylation: An Ab Initio Study. Journal of Physical Chemistry C, 2021, 125, 16316-16323.	1.5	3
5	FAIR Metadata Standards for Low Carbon Energy Researchâ€"A Review of Practices and How to Advance. Energies, 2021, 14, 6692.	1.6	6
6	Non-Equilibrium Green Functions Approach to Study Transport Through a-Si:H/c-Si Interfaces. , 2021, , .		0
7	Semiconductivity Transition in Silicon Nanowires by Hole Transport Layer. Nano Letters, 2020, 20, 8369-8374.	4.5	17
8	Fast Access to Remote Objects 2.0 a renewed gateway to ENEAGRID distributed computing resources. Future Generation Computer Systems, 2019, 94, 920-928.	4.9	10
9	Computational characterization of a-Si:H/c-Si interfaces. Journal of Computational Electronics, 2018, 17, 1457-1469.	1.3	3
10	Ab initio study on localization and finite size effects in the structural, electronic, and optical properties of hydrogenated amorphous silicon. Computational Materials Science, 2018, 155, 159-168.	1.4	7
11	Ab-initio study of hydrogen mobility in the vicinity of MgH2Mg interface: The role of Ti and TiO2. Journal of Alloys and Compounds, 2017, 696, 548-559.	2.8	11
12	Biomembrane solubilization mechanism by Triton X-100: a computational study of the three stage model. Physical Chemistry Chemical Physics, 2017, 19, 29780-29794.	1.3	39
13	Ab Initio Description of Optoelectronic Properties at Defective Interfaces in Solar Cells. Lecture Notes in Computer Science, 2017, , 111-124.	1.0	2
14	Towards a Multi-scale Approach to the Simulation of Silicon Hetero-junction Solar Cells. Journal of Green Engineering (discontinued), 2016, 5, 11-32.	0.7	3
15	Crystal-Like Rearrangements of Icosahedra in Simulated Copper-Zirconium Metallic Glasses and their Effect on Mechanical Properties. Physical Review Letters, 2015, 115, 165501.	2.9	32
16	Molecular dynamics of ionic self-diffusion at an MgO grain boundary. Journal of Materials Science, 2015, 50, 2502-2509.	1.7	21
17	The role of nickel catalyst in hydrogen desorption from MgH 2 : A DFT study. International Journal of Hydrogen Energy, 2015, 40, 9326-9334.	3.8	15
18	Molecular dynamics simulation of corrosion mitigation of iron in lead-bismuth eutectic using nitrogen as corrosion inhibitor. Journal of Physics: Conference Series, 2015, 622, 012009.	0.3	10

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19	Adsorption of Modified Arg, Lys, Asp, and Gln to Dry and Hydrated ZnO Surface: A Density Functional Theory Study. Journal of Physical Chemistry B, 2015, 119, 11791-11797.	1.2	13
20	Self-Assembly of Triton X-100 in Water Solutions: A Multiscale Simulation Study Linking Mesoscale to Atomistic Models. Journal of Chemical Theory and Computation, 2015, 11, 4959-4971.	2.3	41
21	Water driven adsorption of amino acids on the (101) anatase TiO₂ surface: an ab initio study. Physical Chemistry Chemical Physics, 2015, 17, 1556-1561.	1.3	34
22	The effects of vacancies in the mechanical properties of tungsten: A first-principles study. Nuclear Instruments & Methods in Physics Research B, 2015, 342, 70-75.	0.6	12
23	Study of iron structure stability in high temperature molten lead-bismuth eutectic with oxygen injection using molecular dynamics simulation. , 2014, , .		3
24	Inhibition of iron corrosion in high temperature stagnant liquid lead: A molecular dynamics study. Annals of Nuclear Energy, 2013, 62, 298-306.	0.9	16
25	DFT model of hydrogen desorption from MgH2: The role of iron catalyst. International Journal of Hydrogen Energy, 2013, 38, 15254-15263.	3.8	25
26	A brief summary of the progress on the EFDA tungsten materials program. Journal of Nuclear Materials, 2013, 442, S173-S180.	1.3	69
27	GCMC simulation of hydrogen adsorption in densely packed arrays of Li-doped and hydrogenated carbon nanotubes. Journal of Nanoparticle Research, 2013, 15, 1.	0.8	4
28	The ideal tensile strength of tungsten and tungsten alloys by first-principles calculations. Journal of Nuclear Materials, 2013, 435, 52-55.	1.3	30
29	Recent progress in research on tungsten materials for nuclear fusion applications in Europe. Journal of Nuclear Materials, 2013, 432, 482-500.	1.3	610
30	Surface States and Electronic Properties for Small Cadmium Sulfide Nanocluster. Nanoscience and Nanotechnology Letters, 2013, 5, 1182-1187.	0.4	0
31	Organic Functionalization of Metal Oxide Surfaces: An Atomic Scale Modeling Approach. Nanoscience and Nanotechnology Letters, 2013, 5, 1147-1154.	0.4	6
32	Numerical study: Iron corrosion-resistance in lead-bismuth eutectic coolant by molecular dynamics method. AIP Conference Proceedings, 2012, , .	0.3	2
33	Hydrogen Desorption from Mg Hydride: An Ab Initio Study. Crystals, 2012, 2, 845-860.	1.0	10
34	Crystalline and liquid Si3N4characterization by ï¬rst-principles molecular dynamics simulations. EPJ Web of Conferences, 2011, 15, 02008.	0.1	0
35	DFT study of interstitial hydrogen in tantalum lattice. International Journal of Hydrogen Energy, 2011, 36, 13858-13865.	3.8	10
36	Pressure effects on icosahedral short range order in undercooled copper. Solid State Sciences, 2010, 12, 179-182.	1.5	1

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37	Numerical Simulation of Hydrogen Dynamics at a Mg-MgH₂Interface. Advances in Science and Technology, 2010, 72, 205-212.	0.2	1
38	First-principles lattice dynamical study of ScAs and ScSb at zero and high pressure. Solid State Communications, 2009, 149, 1326-1329.	0.9	6
39	Atomic structure of the two intermediate phase glasses<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow><mml:mtext>SiSe</mml:mtext></mml:mrow><mml:mn>4</mml:mn></mml:msub></mml:mrow></mml:math> and<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow><mml:mtext>GeSe</mml:mtext></mml:mrow><mml:mn>4</mml:mn></mml:msub></mml:mrow></mml:math>. Physical Review B, 2009, 79, .	1.1	61
40	Atomic-Scale Modeling of the Interaction between Short Polypeptides and Carbon Surfaces. Journal of Physical Chemistry B, 2009, 113, 12105-12112.	1.2	34
41	Hydrogen Storage in MgH₂ Matrices: An Ab-Initio Study of Mg-MgH₂ Interface. Solid State Phenomena, 2008, 139, 23-28.	0.3	4
42	Experimental and Theoretical Characterization of the 3D-Dopants Bias on the H Desorption of Mg Hydrides. Materials Science Forum, 2007, 555, 349-354.	0.3	6
43	Role of defective icosahedra in undercooled copper. Physical Review B, 2007, 75, .	1.1	24
44	First principles modeling of intermediate range order in amorphous SiSe2. Computational Materials Science, 2005, 33, 106-111.	1.4	1
45	Charge fluctuations and concentration fluctuations at intermediate-range distances in the disordered network-forming materialsSiO2,SiSe2, andGeSe2. Physical Review B, 2004, 70, .	1.1	38
46	Origin of Network Connectivity and Structural Units in AmorphousSiSe2. Physical Review Letters, 2003, 90, 125502.	2.9	25
47	Evidence of concentration fluctuations in disordered network-forming systems: the case of GeSe4and SiSe2. Journal of Physics Condensed Matter, 2003, 15, S1537-S1546.	0.7	6
48	Strain maps at the atomic scale below Ge pyramids and domes on a Si substrate. Applied Physics Letters, 2002, 80, 3736-3738.	1.5	33
49	Point defects and stacking faults in TiSi2phases by tight binding molecular dynamics. Journal of Physics Condensed Matter, 2002, 14, 9535-9553.	0.7	11
50	Atomic hydrogen adsorption on a Stoneâ€“Wales defect in graphite. Surface Science, 2002, 496, 33-38.	0.8	55
51	Beyond short-range order length scales in disordered materials: first principles modeling of SiSe2. Computational Materials Science, 2002, 24, 28-32.	1.4	2
52	2D versus 3D competition at the early stages of growth for Ge on Si(001) by molecular dynamics. Materials Science and Engineering B: Solid-State Materials for Advanced Technology, 2002, 89, 157-159.	1.7	1
53	Atomistic simulation of liquid lead and leadâ€“bismuth eutectic. Journal of Nuclear Materials, 2002, 301, 64-69.	1.3	14
54	First principles investigation of the intermediate range order in disordered materials: the case of SiSe2. Computer Physics Communications, 2002, 147, 166-169.	3.0	2

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55	Thermodynamic behavior of a carbon schwarzite. Computational Materials Science, 2001, 20, 387-393.	1.4	7
56	Ab-initio modelling of atomic and molecular Hydrogen adsorption in graphite. Materials Research Society Symposia Proceedings, 2001, 677, 4111.	0.1	0
57	Ab-initio modelling of atomic and molecular Hydrogen adsorption in graphite. Materials Research Society Symposia Proceedings, 2001, 677, 471.	0.1	1
58	Silicon diffusion in competitive TiSi2 phases by molecular dynamics simulations. Microelectronic Engineering, 2001, 55, 83-92.	1.1	7
59	Static atomic displacements in Ni-rich Ni-Al. Europhysics Letters, 2001, 54, 482-487.	0.7	5
60	Molecular dynamics characterization of crystalline and amorphous TiSi2 phases. Microelectronic Engineering, 2000, 50, 171-177.	1.1	2
61	Structural and thermoelastic properties of crystalline and amorphousTiSi2phases by tight-binding molecular dynamics. Physical Review B, 2000, 61, 14405-14413.	1.1	16
62	Thermodynamic properties of amorphous silicon via tight binding simulations. Computational Materials Science, 2000, 17, 374-379.	1.4	2
63	Neutral and anionic CuO2: an ab inito study. Computational Materials Science, 2000, 17, 539-543.	1.4	13
64	Assessing the driving force of a structural distortion by the simulated evolution of the local density of states. Physical Review B, 1999, 59, 3480-3488.	1.1	14
65	Tight binding simulation of the thermodynamic behavior of amorphous silicon. Journal of Applied Physics, 1999, 86, 6826-6834.	1.1	15
66	An high performance Fortran implementation of a Tight-Binding Molecular Dynamics simulation. Computer Physics Communications, 1999, 120, 255-268.	3.0	4
67	Supersoft elastic parameters and low melting temperature of the C49 phase in TiSi2 by Brillouin scattering and molecular dynamics. Applied Physics Letters, 1999, 74, 3654-3656.	1.5	18
68	Thermodynamic behavior of the carbon schwarzite fcc(C36)2. Physical Review B, 1999, 60, 16928-16933.	1.1	42
69	Self-organized layered structure in epitaxially stabilized FeSi. Europhysics Letters, 1997, 37, 139-144.	0.7	8
70	Analysis of the metal-semiconductor structural phase transition in FeSi 2 by tight-binding molecular dynamics. Europhysics Letters, 1997, 37, 415-420.	0.7	8
71	Mechanical Instability of Oxidized Metal Clusters. Physical Review Letters, 1996, 77, 2495-2498.	2.9	10
72	Atomic model of a palladium nanostructure. Materials Science & Engineering A: Structural Materials: Properties, Microstructure and Processing, 1995, 204, 101-106.	2.6	6

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73	Atomic simulation of a palladium nanophase. Scripta Materialia, 1995, 6, 751-754.	0.5	8
74	Atomic Scale Modelling of Materials: A Prerequisite for any Multi-Scale Approach to Structural and Dynamical Properties. Solid State Phenomena, 0, 139, 141-150.	0.3	0
75	Metallographic and Numerical Studies of the Role of Catalyst Particles of MgH₂-Mg System. Defect and Diffusion Forum, 0, 297-301, 263-268.	0.4	1