Olivier Politano

List of Publications by Year
in descending order

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60 papers	1,231 citations	331259 21 h-index	377514 34 g-index
60 all docs	60 docs citations	60 times ranked	957 citing authors

#	Article	IF	Citations
1	Structure evolution and reaction mechanism in the Ni/Al reactive multilayer nanofoils. Acta Materialia, 2014, 66, 86-96.	3.8	87
2	Reactive Molecular Dynamics of the Initial Oxidation Stages of Ni(111) in Pure Water: Effect of an Applied Electric Field. Journal of Physical Chemistry A, 2012, 116, 11796-11805.	1.1	78
3	Energetics of hydrogen impurities in aluminum and their effect on mechanical properties. Physical Review B, 2002, 65, .	1.1	75
4	Combustion in reactive multilayer Ni/Al nanofoils: Experiments and molecular dynamic simulation. Combustion and Flame, 2016, 166, 158-169.	2.8	73
5	Molecular dynamics simulations of the nano-scale room-temperature oxidation of aluminum single crystals. Surface Science, 2005, 579, 47-57.	0.8	67
6	Molecular dynamics simulations of nanometric metallic multilayers: Reactivity of the Ni-Al system. Physical Review B, 2011, 84, .	1.1	57
7	Nanoscale oxide growth on Al single crystals at low temperatures: Variable charge molecular dynamics simulations. Physical Review B, 2006, 73, .	1.1	54
8	Effects of planetary ball milling on AlCoCrFeNi high entropy alloys prepared by Spark Plasma Sintering: Experiments and molecular dynamics study. Journal of Alloys and Compounds, 2020, 820, 153448.	2.8	49
9	Dissolution process at solid/liquid interface in nanometric metallic multilayers: Molecular dynamics simulations versus diffusion modeling. Acta Materialia, 2015, 99, 363-372.	3.8	46
10	Variable-charge method applied to study coupled grain boundary migration in the presence of oxygen. Acta Materialia, 2009, 57, 1988-2001.	3.8	45
11	Microstructure development during NiAl intermetallic synthesis in reactive Niâ€“Al nanolayers: Numerical investigations vs. TEM observations. Surface and Coatings Technology, 2013, 215, 485-492.	2.2	43
12	Diffusion of oxygen in nickel: A variable charge molecular dynamics study. Solid State Communications, 2010, 150, 439-442.	0.9	42
13	SHS in Ni/Al Nanofoils: A Review of Experiments and Molecular Dynamics Simulations. Advanced Engineering Materials, 2018, 20, 1800091.	1.6	38
14	Combustion synthesis of TiC-based ceramic-metal composites with high entropy alloy binder. Journal of the European Ceramic Society, 2020, 40, 2527-2532.	2.8	35
15	Modeling self-sustaining waves of exothermic dissolution in nanometric Ni-Al multilayers. Acta Materialia, 2016, 120, 189-204.	3.8	31
16	Comparative study of embedded-atom methods applied to the reactivity in the Niâ€“Al system. Modelling and Simulation in Materials Science and Engineering, 2017, 25, 064002.	0.8	28
17	Alloying propagation in nanometric Ni/Al multilayers: A molecular dynamics study. Journal of Applied Physics, 2017, 121, .	1.1	27
18	Oxidation of nanocrystalline aluminum by variable charge molecular dynamics. Journal of Physics and Chemistry of Solids, 2010, 71, 119-124.	1.9	26

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19	Epitaxial growth of the intermetallic compound NiAl on low-index Ni surfaces in Ni/Al reactive multilayer nanofoils. Acta Materialia, 2018, 148, 133-146.	3.8	24
20	Electrochemical properties of crystallized dilithium squarate: insight from dispersion-corrected density functional theory. Physical Chemistry Chemical Physics, 2012, 14, 11398.	1.3	23
21	Molecular dynamics simulations of self-propagating reactions in Niâ€“Al multilayer nanofoils. Journal of Alloys and Compounds, 2015, 652, 25-29.	2.8	22
22	A local chemical potential approach within the variable charge method formalism. Modelling and Simulation in Materials Science and Engineering, 2008, 16, 025006.	0.8	18
23	Grain size, stress and surface roughness. Surface and Interface Analysis, 2008, 40, 518-521.	0.8	17
24	Microstructure evolution and self-propagating reactions in Ni-Al nanofoils: An atomic-scale description. Journal of Alloys and Compounds, 2017, 708, 989-998.	2.8	17
25	A 3D mesoscopic approach for discrete dislocation dynamics. Materials Science & Engineering A: Structural Materials: Properties, Microstructure and Processing, 2001, 309-310, 261-264.	2.6	13
26	An empirical method to determine the free surface energy of solids at different deformations and temperature regimes: An application to Al. Surface Science, 2005, 586, 15-24.	0.8	13
27	A variable charge molecular dynamics study of the initial stage of nickel oxidation. Applied Surface Science, 2010, 256, 5968-5972.	3.1	13
28	Electronic structure and energy decomposition analyses as a tool to interpret the redox potential ranking of naphtho-, biphenyl- and biphenylene-quinone isomers. Physical Chemistry Chemical Physics, 2016, 18, 26651-26660.	1.3	13
29	ReaxFF molecular dynamics simulation study of nanoelectrode lithography oxidation process on silicon (100) surface. Applied Surface Science, 2019, 496, 143679.	3.1	12
30	Self-propagating waves of crystallization in metallic glasses. Applied Physics Letters, 2017, 111, 093105.	1.5	11
31	High-Entropy-Alloy Binder for TiC-Based Cemented Carbide by SHS Method. International Journal of Self-Propagating High-Temperature Synthesis, 2019, 28, 196-198.	0.2	11
32	Reactivity of the Tiâ€“Al system: Experimental study and molecular dynamics simulations. Journal of Applied Physics, 2020, 127, .	1.1	11
33	Reaction front propagation in nanocrystalline Ni/Al composites: A molecular dynamics study. Journal of Applied Physics, 2020, 128, .	1.1	11
34	Molecular dynamics study of high-pressure alumina polymorphs with a tight-binding variable-charge model. Computational Materials Science, 2016, 111, 181-189.	1.4	9
35	Explosive crystallization in amorphous CuTi thin films: a molecular dynamics study. Journal of Non-Crystalline Solids, 2019, 505, 202-210.	1.5	8
36	Mechanical alloying in the Co-Fe-Ni powder mixture: Experimental study and molecular dynamics simulation. Powder Technology, 2022, 399, 117187.	2.1	8

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37	On the dynamics of dislocation patterning. Materials Science & Engineering A: Structural Materials: Properties, Microstructure and Processing, 1997, 234-236, 397-400.	2.6	7
38	Numerical and theoretical considerations on the surface energy for pure solids under strain. Materials Science & Engineering A: Structural Materials: Properties, Microstructure and Processing, 2004, 387-389, 749-752.	2.6	7
39	Thermal Stability of Medium- and High-Entropy Alloys of 3d-Transition Metals. Journal of Phase Equilibria and Diffusion, 2021, 42, 720-734.	0.5	7
40	Formation of surface roughness on nanocrystalline aluminium samples under straining by molecular dynamics studies. Philosophical Magazine, 2007, 87, 129-145.	0.7	6
41	A Reactive Force Field Molecular Dynamics Simulation Study of Corrosion of Nickel. Defect and Diffusion Forum, 0, 323-325, 139-145.	0.4	6
42	An empirical model for free surface energy of strained solids at different temperature regimes. Applied Surface Science, 2006, 252, 5384-5386.	3.1	5
43	Molecular Dynamics Studies in Nanojoining: Self-Propagating Reaction in Ni/Al Nanocomposites. Journal of Materials Engineering and Performance, 2021, 30, 3160-3166.	1.2	5
44	Effects of mechanical activation on chemical homogeneity and contamination level in dual-phase AlCoCrFeNi high entropy alloy. Materials Chemistry and Physics, 2021, 272, 125000.	2.0	5
45	Theoretical and numerical considerations on the surface energy for deformed isotropic nanocrystals. Philosophical Magazine, 2004, 84, 3397-3409.	0.7	4
46	Reactivity of Niâ€“Al nanocomposites prepared by mechanical activation: A molecular dynamics study. Journal of Applied Physics, 2021, 129, 065301.	1.1	4
47	Dynamical features of forest interactions. Computational Materials Science, 2000, 17, 343-346.	1.4	3
48	Dissolution at Interfaces in Layered Solid-Liquid Thin Films: A Key Step in Joining Process. Journal of Materials Engineering and Performance, 2016, 25, 3270-3274.	1.2	3
49	Substrate orientation effects on nanoelectrode lithography: ReaxFF molecular dynamics and experimental study. Journal Physics D: Applied Physics, 2020, 53, 295108.	1.3	3
50	Numerical Determination of Intrinsic Diffusion Coefficient of Aluminide Coatings on Metals. Defect and Diffusion Forum, 0, 289-292, 269-276.	0.4	2
51	Numerical Simulations on the Growth of Thin Oxide Films on Aluminum Substrates. Defect and Diffusion Forum, 2010, 297-301, 954-959.	0.4	2
52	Numerical Studies of the Diffusion Processes and First Step Oxidation in Nickel-Oxygen Systems by Variable Charge Molecular Dynamics. Defect and Diffusion Forum, 2010, 297-301, 513-518.	0.4	2
53	Mechanical activation of metallic powders in planetary ball mills: multi-scale modeling and experimental observation. IOP Conference Series: Materials Science and Engineering, 2019, 558, 012034.	0.3	2
54	Determination of the Stress Distribution at the Interface Metal-Oxide: Numerical and Theoretical Considerations. Defect and Diffusion Forum, 2005, 237-240, 145-150.	0.4	1

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55	Quenched molecular dynamics studies on the extraction energy of aluminum atoms. Surface and Interface Analysis, 2008, 40, 320-322.	0.8	1
56	Mechanical activation of metallic powders and reactivity of activated nanocomposites: a molecular dynamics approach. Applied Physics A: Materials Science and Processing, 2021, 127, 1.	1.1	1
57	Numerical Determination of Intrinsic Diffusion in Fe-Cr-Al Systems. Defect and Diffusion Forum, 2010, 297-301, 948-953.	0.4	0
58	Study of the Reactive Dynamics of Nanometric Metallic Multilayers Using Molecular Dynamics : The Al-Ni System. Defect and Diffusion Forum, 0, 323-325, 89-94.	0.4	0
59	Preface for MMM 2016 focus issue. Modelling and Simulation in Materials Science and Engineering, 2018, 26, 010301.	0.8	0
60	Molecular Dynamics Simulation of Self-Propagating Thermal Waves in Amorphous Cu50Ti50 Films and Thin Cu/Ti Sandwiches. International Journal of Self-Propagating High-Temperature Synthesis, 2018, 27, 114-116.	0.2	0