Davide G Sangiovanni

List of Publications by Year
in descending order

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55 papers	2,125 citations	159585 30 h-index	233421 45 g-index
56 all docs	56 docs citations	56 times ranked	1407 citing authors

#	Article	IF	Citations
1	Supertoughening in B1 transition metal nitride alloys by increased valence electron concentration. Acta Materialia, 2011, 59, 2121-2134. Electronic mechanism for toughness enhancement in<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"	7.9	166
2			

#	Article	IF	Citations
19	Effect of WN content on toughness enhancement in V1â^'xWxN/MgO(001) thin films. Journal of Vacuum Science and Technology A: Vacuum, Surfaces and Films, 2014, 32, .	2.1	45
20	Elastic properties and plastic deformation of TiC- and VC-based pseudobinary alloys. Acta Materialia, 2018, 144, 376-385.	7.9	45
21	Ti adatom diffusion on TiN(001): Ab initio and classical molecular dynamics simulations. Surface Science, 2014, 627, 34-41.	1.9	40
22	Ab Initio Molecular Dynamics Simulations of Nitrogen/VN(001) Surface Reactions: Vacancy-Catalyzed N₂ Dissociative Chemisorption, N Adatom Migration, and N₂ Desorption. Journal of Physical Chemistry C, 2016, 120, 12503-12516.	3.1	39
23	Atomic-scale diffusion rates during growth of thin metal films on weakly-interacting substrates. Scientific Reports, 2019, 9, 6640.	3.3	35
24	Effects of atomic ordering on the elastic properties of TiN- and VN-based ternary alloys. Thin Solid Films, 2014, 571, 145-153.	1.8	34
25	Experimental and computational studies on toughness enhancement in Ti-Al-Ta-N quaternaries. Journal of Vacuum Science and Technology A: Vacuum, Surfaces and Films, 2017, 35, .	2.1	34
26	Phonon and electron contributions to the thermal conductivity of <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:mi mathvariant="normal">V</mml:mi><mml:msub><mml:mi mathvariant="normal">N</mml:mi><mml:mi>x</mml:mi></mml:msub></mml:mrow></mml:math> epitaxial layers. Physical Review Materials, 2017, 1, .	2.4	34
27	N and Ti adatom dynamics on stoichiometric polar TiN(111) surfaces. Surface Science, 2016, 649, 72-79.	1.9	32
28	Enhancing plasticity in high-entropy refractory ceramics via tailoring valence electron concentration. Materials and Design, 2021, 209, 109932.	7.0	32
29	Effects of incident N atom kinetic energy on TiN/TiN(001) film growth dynamics: A molecular dynamics investigation. Journal of Applied Physics, 2017, 121, .	2.5	31
30	Large-scale molecular dynamics simulations of TiN/TiN(001) epitaxial film growth. Journal of Vacuum Science and Technology A: Vacuum, Surfaces and Films, 2016, 34, .	2.1	30
31	Growth, nanostructure, and optical properties of epitaxial VN_x/MgO(001) (0.80 â‰¤ x â‰¤ 1.00) layers deposited by reactive magnetron sputtering. Journal of Materials Chemistry C, 2016, 4, 7924-7938.	5.5	30
32	Ti and N adatom descent pathways to the terrace from atop two-dimensional TiN/TiN(001) islands. Thin Solid Films, 2014, 558, 37-46.	1.8	29
33	Atomistic mechanisms underlying plasticity and crack growth in ceramics: a case study of AlN/TiN superlattices. Acta Materialia, 2022, 229, 117809.	7.9	29
34	Superionic‐like Diffusion in an Elemental Crystal: bcc Titanium. Physical Review Letters, 2019, 123, 105501.	7.8	28
35	Temperature-dependent elastic properties of binary and multicomponent high-entropy refractory carbides. Materials and Design, 2021, 204, 109634.	7.0	26
36	Effect of dispersion corrections on ab initio predictions of graphite and diamond properties under pressure. Physical Review B, 2018, 98, .	3.2	24

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37	Semi-Empirical Force-Field Model for the Ti1â‾xAlxN (0 â‰¤ x â‰¤ 1) System. Materials, 2019, 12, 215.	2.9	22
38	Effects of surface vibrations on interlayer mass transport: Ab initio molecular dynamics investigation of Ti adatom descent pathways and rates from TiN/TiN(001) islands. Physical Review B, 2018, 97, .	3.2	21
39	Predicting elastic properties of hard-coating alloys using ab-initio and machine learning methods. Npj Computational Materials, 2022, 8, .	8.7	16
40	Nonequilibrium ab initio molecular dynamics determination of Ti monovacancy migration rates in <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:mi>B</mml:mi><mml:mn>1</mml:mn></mml:mrow></mml:m TiN. Physical Review B, 2017, 96, .	3.2	15
41	Adsorption-controlled growth and properties of epitaxial SnO films. Physical Review Materials, 2019, 3, .	2.4	15
42	Thermally induced age hardening in tough Ta-Al-N coatings via spinodal decomposition. Journal of Applied Physics, 2017, 121, .	2.5	14
43	Anomalous versus Normal Room-Temperature Diffusion of Metal Adatoms on Graphene. Journal of Physical Chemistry Letters, 2020, 11, 8930-8936.	4.6	14
44	Atomistic description of self-diffusion in molybdenum: A comparative theoretical study of non-Arrhenius behavior. Physical Review Materials, 2020, 4, .	2.4	14
45	The dynamics of TiNx (x = 1â€“3) admolecule interlayer and intralayer transport on TiN/TiN(001) islands. Thin Solid Films, 2015, 589, 133-144.	1.8	12
46	Copper adatom, admolecule transport, and island nucleation on TiN(0â€¯0â€¯1) via ab initio molecular dynamics. Applied Surface Science, 2018, 450, 180-189.	6.1	12
47	First-principles characterization of reversible martensitic transformations. Physical Review B, 2019, 99, .	3.2	12
48	Strength, transformation toughening, and fracture dynamics of rocksalt-structure <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:mi mathvariant="normal">T</mml:mi><mml:msub><mml:mi mathvariant="normal">i</mml:mi><mml:mrow><mml:mn>1</mml:mn><mml:mo>â‾</mml:mo><mml:mi>x</mml:mi></mml:mrow></m mathvariant="normal">A</mml:mi><mml:msub><mml:mi mathvariant="normal">l</mml:mi><mml:mi>x</mml:mi></mml:msub><mml:mi mathvariant="normal">N	2.4	12
49	Efficient and accurate determination of lattice-vacancy diffusion coefficients via non equilibriumab initiomolecular dynamics. Physical Review B, 2016, 93, .	3.2	11
50	Thermally induced structural evolution and age-hardening of polycrystalline V1â€“xMoxN (xÂâ‰ˆÂ0.4) thin films. Surface and Coatings Technology, 2021, 405, 126723.	4.8	11
51	TiN film growth on misoriented TiN grains with simultaneous low-energy bombardment: Restructuring leading to epitaxy. Thin Solid Films, 2019, 688, 137380.	1.8	7
52	Mass transport properties of quasiharmonic vs. anharmonic transition-metal nitrides. Thin Solid Films, 2019, 688, 137297.	1.8	7
53	Room-temperature diffusion of metal clusters on graphene. Physical Chemistry Chemical Physics, 2021, 23, 13087-13094.	2.8	6
54	Color and pseudogap tunability in multicomponent carbonitrides. Materials and Design, 2022, 217, 110600.	7.0	2

#	Article	IF	Citations
55	Mechanical properties of VMoNO as a function of oxygen concentration: Toward development of hard and tough refractory oxynitrides. Journal of Vacuum Science and Technology A: Vacuum, Surfaces and Films, 2019, 37, .	2.1	1