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The third column is the impact factor (IF) of the journal, and the fourth column is the number of citations of the article.

45 papers	747 citations	17 h-index	26 g-index
51 ext. papers	802 ext. citations	3.1 avg, IF	3.92 L-index

#	Paper	IF	Citations
45	Theoretical study of dislocation nucleation from simple surface defects in semiconductors. <i>Physical Review B</i> , 2004 , 70,	3.3	70
44	Proton diffusion mechanism in amorphous SiO ₂ . <i>Physical Review Letters</i> , 2006 , 97, 155901	7.4	54
43	Elastic limit for surface step dislocation nucleation in face-centered cubic metals: Temperature and step height dependence. <i>Acta Materialia</i> , 2010 , 58, 4182-4190	8.4	48
42	Dislocation formation from a surface step in semiconductors: An ab initio study. <i>Physical Review B</i> , 2006 , 73,	3.3	41
41	A new parametrization of the Stillinger-Weber potential for an improved description of defects and plasticity of silicon. <i>Journal of Physics Condensed Matter</i> , 2013 , 25, 055801	1.8	40
40	First principles investigation of defect energy levels at semiconductor-oxide interfaces: Oxygen vacancies and hydrogen interstitials in the Si/SiO ₂ /HfO ₂ stack. <i>Journal of Applied Physics</i> , 2009 , 105, 061603	2.5	38
39	Glissile dislocations with transient cores in silicon. <i>Physical Review Letters</i> , 2009 , 103, 065505	7.4	36
38	Comparison between classical potentials and ab initio methods for silicon under large shear. <i>Journal of Physics Condensed Matter</i> , 2003 , 15, 6943-6953	1.8	35
37	Deformation of silicon nanowires studied by molecular dynamics simulations. <i>Modelling and Simulation in Materials Science and Engineering</i> , 2011 , 19, 074003	2	22
36	Determination of activation parameters for dislocation formation from a surface in fcc metals by atomistic simulations. <i>Physical Review B</i> , 2008 , 78,	3.3	22
35	Hydrogen in Si(100)/SiO ₂ /HfO ₂ gate stacks: Relevant charge states and their location. <i>Applied Physics Letters</i> , 2007 , 91, 262901	3.4	21
34	Plasticity in crystalline-amorphous core-shell Si nanowires controlled by native interface defects. <i>Physical Review B</i> , 2013 , 87,	3.3	20
33	Proton-induced fixed positive charge at the Si(100)-SiO ₂ interface. <i>Physical Review Letters</i> , 2007 , 99, 126102	7.4	20
32	Ab initio study of charged states of H in amorphous SiO ₂ . <i>Microelectronic Engineering</i> , 2005 , 80, 288-291	2.5	20
31	Computer study of microtwins forming from surface steps of silicon. <i>Computational Materials Science</i> , 2004 , 30, 16-20	3.2	19
30	Low-temperature intrinsic plasticity in silicon at small scales. <i>Acta Materialia</i> , 2018 , 161, 54-60	8.4	19
29	Unexpected slip mechanism induced by the reduced dimensions in silicon nanostructures: Atomistic study. <i>Acta Materialia</i> , 2011 , 59, 7464-7472	8.4	17

28	Atomistic simulations of $\langle 110 \rangle$ screw dislocation core in magnesium oxide. <i>Computational Materials Science</i> , 2015 , 103, 250-255	3.2	16
27	Dislocation nucleation from surface step in silicon: The glide set versus the shuffle set. <i>Physica Status Solidi (A) Applications and Materials Science</i> , 2009 , 206, 1885-1891	1.6	15
26	Onset of ductility and brittleness in silicon nanowires mediated by dislocation nucleation. <i>Modelling and Simulation in Materials Science and Engineering</i> , 2015 , 23, 025010	2	13
25	Properties of threading screw dislocation core in wurtzite GaN studied by Heyd-Scuseria-Ernzerhof hybrid functional. <i>Applied Physics Letters</i> , 2013 , 103, 262107	3.4	13
24	MgO/metal interfaces at low coverage: An order N, semiempirical Hartree-Fock simulation. <i>Physical Review B</i> , 2010 , 81,	3.3	12
23	Uniform tensile elongation in Au@Si core-shell nanowires. <i>Extreme Mechanics Letters</i> , 2016 , 8, 151-159	3.9	11
22	Surface effects on the mechanical behavior of silicon nanowires: Consequence on the brittle to ductile transition at low scale and low temperature. <i>Physica Status Solidi (A) Applications and Materials Science</i> , 2015 , 212, 1643-1648	1.6	10
21	Determination of activation parameters for the core transformation of the screw dislocation in silicon. <i>Modelling and Simulation in Materials Science and Engineering</i> , 2010 , 18, 065001	2	10
20	A fully molecular dynamics-based method for modeling nanoporous gold. <i>Computational Materials Science</i> , 2019 , 161, 135-142	3.2	9
19	Surface step effects on Si (100) under uniaxial tensile stress, by atomistic calculations. <i>Scripta Materialia</i> , 2002 , 47, 481-486	5.6	9
18	Theoretical study of hydrogen stability and aggregation in dislocation cores in silicon. <i>Physical Review B</i> , 2010 , 82,	3.3	8
17	Dislocation cores in silicon: new aspects from numerical simulations. <i>Journal of Physics: Conference Series</i> , 2011 , 281, 012002	0.3	7
16	Investigation of the interaction between hydrogen and screw dislocation in silicon by first-principles calculations. <i>Journal of Physics Condensed Matter</i> , 2010 , 22, 035803	1.8	5
15	Protons at the Si-SiO ₂ interface: a first principle investigation. <i>Microelectronic Engineering</i> , 2007 , 84, 2035-2038	2.5	3
14	Molecular dynamics study of mechanical behavior of gold-silicon core-shell nanowires under cyclic loading. <i>Materialia</i> , 2019 , 5, 100204	3.2	3
13	Propagation of stacking faults from Σ 5 composite dislocation cores at low temperature in silicon nanostructures. <i>Journal of Physics: Conference Series</i> , 2019 , 1190, 012007	0.3	2
12	Influence of strain on dislocation core in silicon. <i>Philosophical Magazine</i> , 2018 , 98, 1151-1169	1.6	2
11	Investigation of Plasticity in Silicon Nanowires by Molecular Dynamics Simulations. <i>Key Engineering Materials</i> , 2011 , 465, 89-92	0.4	2

10	Proton Diffusion in Amorphous SiO ₂ and Hafnium Silicate by Ab Initio Molecular Dynamics. <i>AIP Conference Proceedings</i> , 2007 ,	0	2
9	Plastic behaviour and deformation mechanisms in silicon nano-objects. <i>Journal of Physics: Conference Series</i> , 2019 , 1190, 012004	0.3	1
8	Stacking fault formation created by plastic deformation at low temperature and small scales in silicon. <i>Physical Review Materials</i> , 2020 , 4,	3.2	1
7	Empirical potential optimization for the investigation of lithiation-delithiation cycles of amorphous Si nanowires. <i>Physical Review Materials</i> , 2020 , 4,	3.2	1
6	Atomic scale mechanisms and brittle to ductile transition at low size in silicon. <i>Materials Today: Proceedings</i> , 2018 , 5, 14693-14704	1.4	1
5	Atomistic Simulation of Dislocation Generation at Surface Steps in Metals and Silicon. <i>Solid Mechanics and Its Applications</i> , 2004 , 129-138	0.4	1
4	Comment on "Bulk dislocation core dissociation probed by coherent x rays in silicon". <i>Physical Review Letters</i> , 2011 , 107, 199601; discussion 199602	7.4	0
3	HRTEM study of structural defects and related deformation mechanisms induced by nanocompression of silicon 2016 , 261-262		
2	A Theoretical Study of Dislocation Formation at Surfaces in Covalent Materials: Effect of Step Geometry and Reactivity. <i>Solid State Phenomena</i> , 2005 , 108-109, 193-198	0.4	
1	Onset of Plasticity in Crystalline Nanomaterials 61-82		