Efthimios Kaxiras

List of Publications by Citations

394 papers	30,187 citations	85 h-index	163 g-index
407 ext. papers	35,262 ext. citations	6.6 avg, IF	7.47 L-index

#	Paper	IF	Citations
394	Unconventional superconductivity in magic-angle graphene superlattices. *Nature*, **2018**, 556, 43-50	50.4	2942
393	Optimized pseudopotentials. *Physical Review B*, **1990**, 41, 1227-1230	3.3	1876
392	Correlated insulator behaviour at half-filling in magic-angle graphene superlattices. *Nature*, **2018**, 556, 80-84	50.4	1771
391	Surfactants in epitaxial growth. *Physical Review Letters*, **1989**, 63, 632-635	7.4	1004
390	Hydrogen bonding and stacking interactions of nucleic acid base pairs: A density-functional-theory based treatment. *Journal of Chemical Physics*, **2001**, 114, 5149-5155	3.9	925
389	A QM/MM Implementation of the Self-Consistent Charge Density Functional Tight Binding (SCC-DFTB) Method. *Journal of Physical Chemistry B*, **2001**, 105, 569-585	3.4	523
388	Graphene/MoS2 hybrid technology for large-scale two-dimensional electronics. *Nano Letters*, **2014**, 14, 3055-63	11.5	472
387	Concurrent coupling of length scales: Methodology and application. *Physical Review B*, **1999**, 60, 2391-2403	3.3	460
386	Graphene nanoFlakes with large spin. *Nano Letters*, **2008**, 8, 241-5	11.5	393
385	Interatomic potential for silicon defects and disordered phases. *Physical Review B*, **1998**, 58, 2539-2550	3.3	360
384	Environment-dependent interatomic potential for bulk silicon. *Physical Review B*, **1997**, 56, 8542-8552	3.3	327
383	Adsorption and diffusion of lithium on layered silicon for Li-ion storage. *Nano Letters*, **2013**, 13, 2258-63	11.5	299
382	MoS Field-Effect Transistor with Sub-10 nm Channel Length. *Nano Letters*, **2016**, 16, 7798-7806	11.5	283
381	Atomic and electronic reconstruction at the van der Waals interface in twisted bilayer graphene. *Nature Materials*, **2019**, 18, 448-453	27	282
380	Lithium-assisted plastic deformation of silicon electrodes in lithium-ion batteries: a first-principles theoretical study. *Nano Letters*, **2011**, 11, 2962-7	11.5	276
379	Spanning the continuum to quantum length scales in a dynamic simulation of brittle fracture. *Europhysics Letters*, **1998**, 44, 783-787	1.6	256
378	Adsorption of boron on Si(111): Its effect on surface electronic states and reconstruction. *Physical Review Letters*, **1989**, 63, 1261-1264	7.4	249

377	Spanning the length scales in dynamic simulation. *Computers in Physics*, **1998**, 12, 538		240
376	Tuning the electronic and chemical properties of monolayer MoS2 adsorbed on transition metal substrates. *Nano Letters*, **2013**, 13, 509-14	11.5	239
375	Generalized-stacking-fault energy surface and dislocation properties of aluminum. *Physical Review B*, **2000**, 62, 3099-3108	3.3	237
374	Superlattice-Induced Insulating States and Valley-Protected Orbits in Twisted Bilayer Graphene. *Physical Review Letters*, **2016**, 117, 116804	7.4	218
373	A structural approach to relaxation in glassy liquids. *Nature Physics*, **2016**, 12, 469-471	16.2	214
372	Topological frustration in graphene nanoflakes: magnetic order and spin logic devices. *Physical Review Letters*, **2009**, 102, 157201	7.4	209
371	Identifying structural flow defects in disordered solids using machine-learning methods. *Physical Review Letters*, **2015**, 114, 108001	7.4	206
370	Ab initio theory of polar semiconductor surfaces. I. Methodology and the (22) reconstructions of GaAs(111). *Physical Review B*, **1987**, 35, 9625-9635	3.3	204
369	Semidiscrete Variational Peierls Framework for Dislocation Core Properties. *Physical Review Letters* , **1997**, 78, 4221-4224	7.4	199
368	Ab initio supercell calculations on nitrogen-vacancy center in diamond: Electronic structure and hyperfine tensors. *Physical Review B*, **2008**, 77,	3.3	192
367	Hydrogen embrittlement of aluminum: the crucial role of vacancies. *Physical Review Letters*, **2005**, 94, 155501	7.4	190
366	A Self-Consistent Charge Density-Functional Based Tight-Binding Scheme for Large Biomolecules. *Physica Status Solidi (B): Basic Research*, **2000**, 217, 357-376	1.3	190
365	Energetics of defects and diffusion mechanisms in graphite. *Physical Review Letters*, **1988**, 61, 2693-2696	7.4	182
364	Natural dyes adsorbed on TiO2 nanowire for photovoltaic applications: enhanced light absorption and ultrafast electron injection. *Nano Letters*, **2008**, 8, 3266-72	11.5	181
363	Mixed finite element and atomistic formulation for complex crystals. *Physical Review B*, **1999**, 59, 235-245	3.3	177
362	Twistronics: Manipulating the electronic properties of two-dimensional layered structures through their twist angle. *Physical Review B*, **2017**, 95,	3.3	171
361	Shape of small silicon clusters. *Physical Review Letters*, **1993**, 71, 727-730	7.4	163
360	Observation of the nonlinear Hall effect under time-reversal-symmetric conditions. *Nature*, **2019**, 565, 337-342	50.4	159

359	Theory of spin-conserving excitation of the N-V(-) center in diamond. *Physical Review Letters*, **2009**, 103, 186404	7.4	158
358	Adaptive-coordinate real-space electronic-structure calculations for atoms, molecules, and solids. *Physical Review B*, **1997**, 55, 10289-10301	3.3	154
357	A density functional study of clean and hydrogen-covered MoO3(010): Electronic structure and surface relaxation. *Journal of Chemical Physics*, **1998**, 109, 6854-6860	3.9	149
356	Structural model of eumelanin. *Physical Review Letters*, **2006**, 97, 218102	7.4	148
355	Electric-field dependence of the effective dielectric constant in graphene. *Nano Letters*, **2013**, 13, 898-902	11.5	147
354	Electrically driven tuning of the dielectric constant in MoS2 layers. *ACS Nano*, **2013**, 7, 10741-6	16.7	146
353	Modeling zinc in biomolecules with the self consistent charge-density functional tight binding (SCC-DFTB) method: applications to structural and energetic analysis. *Journal of Computational Chemistry*, **2003**, 24, 565-81	3.5	146
352	Reactive flow in silicon electrodes assisted by the insertion of lithium. *Nano Letters*, **2012**, 12, 4397-403	11.5	145
351	Surfactant mediated crystal growth of semiconductors. *Physical Review Letters*, **1995**, 75, 2742-2745	7.4	145
350	DNA nucleoside interaction and identification with carbon nanotubes. *Nano Letters*, **2007**, 7, 45-50	11.5	144
349	Effect of surface reconstruction on stability and reactivity of Si clusters. *Physical Review Letters*, **1990**, 64, 551-554	7.4	142
348	Free energies of generalized stacking faults in Si and implications for the brittle-ductile transition. *Physical Review Letters*, **1993**, 70, 3752-3755	7.4	139
347	Diffusion of Lithium in Bulk Amorphous Silicon: A Theoretical Study. *Journal of Physical Chemistry C*, **2012**, 116, 22212-22216	3.8	138
346	Adaptive nudged elastic band approach for transition state calculation. *Journal of Chemical Physics*, **2002**, 117, 4651-4658	3.9	138
345	Size limits on doping phosphorus into silicon nanocrystals. *Nano Letters*, **2008**, 8, 596-600	11.5	137
344	Carbon nanotube interaction with DNA. *Nano Letters*, **2005**, 5, 897-900	11.5	136
343	Quantum mechanics simulation of protein dynamics on long timescale. *Proteins: Structure, Function and Bioinformatics*, **2001**, 44, 484-9	4.2	127
342	Heterointerface effects in the electrointercalation of van der Waals heterostructures. *Nature*, **2018**, 558, 425-429	50.4	125

341	Dirac fermions and flat bands in the ideal kagome metal FeSn. *Nature Materials*, **2020**, 19, 163-169	27	121
340	Microscopic theory of electromigration on semiconductor surfaces. *Physical Review Letters*, **1996**, 76, 1114-1117	7.4	118
339	Electron and hole dynamics in dye-sensitized solar cells: influencing factors and systematic trends. *Nano Letters*, **2010**, 10, 1238-47	11.5	116
338	Electronic structure theory of weakly interacting bilayers. *Physical Review B*, **2016**, 93,	3.3	114
337	New Insights into the Structure of the Vapor/Water Interface from Large-Scale First-Principles Simulations. *Journal of Physical Chemistry Letters*, **2011**, 2, 105-13	6.4	114
336	Hydrogen-enhanced local plasticity in aluminum: an ab initio study. *Physical Review Letters*, **2001**, 87, 095501	7.4	112
335	Ab initio tight-binding Hamiltonian for transition metal dichalcogenides. *Physical Review B*, **2015**, 92,	3.3	111
334	Multiscale simulation of loading and electrical resistance in silicon nanoindentation. *Physical Review Letters*, **2000**, 84, 1260-3	7.4	109
333	Metal-diboride nanotubes as high-capacity hydrogen storage media. *Nano Letters*, **2007**, 7, 663-7	11.5	108
332	Optoelectronic properties of single-layer, double-layer, and bulk tin sulfide: A theoretical study. *Journal of Applied Physics*, **2013**, 113, 233507	2.5	107
331	Evidence for trimer reconstruction of Si(111) sqrt 3 x sqrt 3 -Sb: Scanning tunneling microscopy and first-principles theory. *Physical Review B*, **1990**, 42, 7230-7233	3.3	106
330	Exact continuum model for low-energy electronic states of twisted bilayer graphene. *Physical Review Research*, **2019**, 1,	3.9	105
329	Energetic, vibrational, and electronic properties of silicon using a nonorthogonal tight-binding model. *Physical Review B*, **2000**, 62, 4477-4487	3.3	104
328	Semiconductor-surface restoration by valence-mending adsorbates: Application to Si(100):S and Si(100):Se. *Physical Review B*, **1991**, 43, 6824-6827	3.3	104
327	Epitaxial growth of molecular crystals on van der waals substrates for high-performance organic electronics. *Advanced Materials*, **2014**, 26, 2812-7	24	103
326	Complexation of flavonoids with iron: structure and optical signatures. *Journal of Physical Chemistry B*, **2008**, 112, 1845-50	3.4	103
325	Pressure dependence of the magic twist angle in graphene superlattices. *Physical Review B*, **2018**, 98,	3.3	103
324	Modeling of Covalent Bonding in Solids by Inversion of Cohesive Energy Curves. *Physical Review Letters*, **1996**, 77, 4370-4373	7.4	102

323	MUPHY: A parallel MUlti PHYsics/scale code for high performance bio-fluidic simulations. *Computer Physics Communications*, **2009**, 180, 1495-1502	4.2	101
322	Ideal crystal stability and pressure-induced phase transition in silicon. *Physical Review B*, **1994**, 50, 14952-14959	3.7	100
321	Diffusion of adsorbate atoms on the reconstructed Si(111) surface. *Surface Science*, **1998**, 396, L261-L266	1.8	98
320	Onset of metallization and related transitions in solid hydrogen. *Physical Review Letters*, **1991**, 67, 1138-1141	7.4	96
319	Electronic states due to surface doping: Si(111) sqrt 3 x sqrt 3B. *Physical Review B*, **1990**, 41, 1262-1265	3.3	95
318	From electrons to finite elements: A concurrent multiscale approach for metals. *Physical Review B*, **2006**, 73,	3.3	93
317	Electronic structure of solid nitromethane: Effects of high pressure and molecular vacancies. *Journal of Chemical Physics*, **2002**, 117, 788-799	3.9	91
316	Generalized stacking fault energy surfaces and dislocation properties of silicon: A first-principles theoretical study. *Philosophical Magazine A: Physics of Condensed Matter, Structure, Defects and Mechanical Properties*, **1996**, 74, 1367-1384		91
315	A flexible high-performance Lattice Boltzmann GPU code for the simulations of fluid flows in complex geometries. *Concurrency Computation Practice and Experience*, **2010**, 22, 1-14	1.4	89
314	A TDDFT study of the optical response of DNA bases, base pairs, and their tautomers in the gas phase. *Journal of Physical Chemistry A*, **2005**, 109, 2373-80	2.8	89
313	Multiscale simulations of silicon nanoindentation. *Acta Materialia*, **2001**, 49, 4089-4101	8.4	88
312	Relaxation and domain formation in incommensurate two-dimensional heterostructures. *Physical Review B*, **2018**, 98,	3.3	87
311	Theoretical models of eumelanin protomolecules and their optical properties. *Biophysical Journal*, **2008**, 94, 2095-105	2.9	86
310	Atomic structure and bonding of boron-induced reconstructions on Si(001). *Physical Review Letters*, **1995**, 74, 403-406	7.4	86
309	Enhancement of interlayer exchange in an ultrathin two-dimensional magnet. *Nature Physics*, **2019**, 15, 1255-1260	16.2	85
308	Multiscale simulations in simple metals: A density-functional-based methodology. *Physical Review B* , **2005**, 71,	3.3	84
307	New low-energy crystal structure for silicon. *Physical Review Letters*, **1991**, 67, 715-718	7.4	83
306	Theoretical Study of O-Assisted Selective Coupling of Methanol on Au(111). *Journal of Physical Chemistry C*, **2011**, 115, 3703-3708	3.8	82

305	Enhancing the Hydrogen Activation Reactivity of Nonprecious Metal Substrates via Confined Catalysis Underneath Graphene. *Nano Letters*, **2016**, 16, 6058-6063	11.5	82
304	Band-structure calculations for semiconductors within generalized-density-functional theory. *Physical Review B*, **1999**, 59, 5536-5543	3.3	81
303	Stress effects on the initial lithiation of crystalline silicon nanowires: reactive molecular dynamics simulations using ReaxFF. *Physical Chemistry Chemical Physics*, **2015**, 17, 3832-40	3.6	80
302	Multiscale Coupling of Molecular Dynamics and Hydrodynamics: Application to DNA Translocation through a Nanopore. *Multiscale Modeling and Simulation*, **2006**, 5, 1156-1173	1.8	80
301	Application of gradient corrections to density-functional theory for atoms and solids. *Physical Review B*, **1993**, 48, 14944-14952	3.3	78
300	Properties of copper (fluoro-)phthalocyanine layers deposited on epitaxial graphene. *Journal of Chemical Physics*, **2011**, 134, 194706	3.9	75
299	Magnetic resonance spectroscopy of an atomically thin material using a single-spin qubit. *Science*, **2017**, 355, 503-507	33.3	74
298	Strain dependence of band gaps and exciton energies in pure and mixed transition-metal dichalcogenides. *Physical Review B*, **2016**, 94,	3.3	72
297	Chlorine adsorption on Au(111): chlorine overlayer or surface chloride?. *Journal of the American Chemical Society*, **2008**, 130, 3560-5	16.4	72
296	Dimer Pairing on the C-Alloyed Si(001) Surface. *Physical Review Letters*, **1999**, 82, 972-975	7.4	72
295	Atomic Oxygen Adsorption on Au(111) Surfaces with Defects. *Journal of Physical Chemistry C*, **2009**, 113, 3232-3238	3.8	71
294	Comment on graphene nanoflakes with large spin: broken-symmetry states. *Nano Letters*, **2008**, 8, 766	11.5	70
293	Direct observation of a long-lived single-atom catalyst chiseling atomic structures in graphene. *Nano Letters*, **2014**, 14, 450-5	11.5	69
292	Design of Dye Acceptors for Photovoltaics from First-Principles Calculations. *Journal of Physical Chemistry C*, **2011**, 115, 9276-9282	3.8	69
291	Hydrogenation of semiconductor surfaces: Si and Ge (111). *Physical Review B*, **1988**, 37, 8842-8848	3.3	68
290	The role of surface and subsurface point defects for chemical model studies on TiO2: a first-principles theoretical study of formaldehyde bonding on rutile TiO2(110). *Chemistry - A European Journal*, **2011**, 17, 4496-506	4.8	66
289	Structure of III-Sb(001) growth surfaces: the role of heterodimers. *Physical Review Letters*, **2000**, 84, 4649-52	7.4	66
288	Berry curvature dipole current in the transition metal dichalcogenides family. *Physical Review B*, **2018**, 98,	3.3	66

287	Theory of Graphene Raman Scattering. *ACS Nano*, **2016**, 10, 2803-18	16.7	65
286	Microalloying for ductility in molybdenum disilicide. *Materials Science & Engineering A: Structural Materials: Properties, Microstructure and Processing*, **1999**, 261, 147-157	5.3	65
285	Amorphous-crystal interface in silicon: A tight-binding simulation. *Physical Review B*, **1998**, 58, 4579-4583	3.3	64
284	Intermittent diffusion on the reconstructed Si(111) surface. *Europhysics Letters*, **1997**, 39, 287-292	1.6	63
283	Hole dynamics in the two-dimensional strong-coupling Hubbard Hamiltonian. *Physical Review B*, **1988**, 38, 866-869	3.3	63
282	Atomistic simulations of solid-phase epitaxial growth in silicon. *Physical Review B*, **2000**, 61, 6696-6700	3.3	62
281	Relationship between local structure and relaxation in out-of-equilibrium glassy systems. *Proceedings of the National Academy of Sciences of the United States of America*, **2017**, 114, 263-267	11.5	60
280	First principles study of point defects in SnS. *Physical Chemistry Chemical Physics*, **2014**, 16, 26176-83	3.6	60
279	Vacancy in Silicon Revisited: Structure and Pressure Effects. *Physical Review Letters*, **1998**, 81, 2088-2091	7.4	60
278	eReaxFF: A Pseudoclassical Treatment of Explicit Electrons within Reactive Force Field Simulations. *Journal of Chemical Theory and Computation*, **2016**, 12, 3463-72	6.4	59
277	Embrittlement of metal by solute segregation-induced amorphization. *Physical Review Letters*, **2010**, 104, 155502	7.4	58
276	Use of the generalized gradient approximation in pseudopotential calculations of solids. *Physical Review B*, **1995**, 51, 9521-9525	3.3	58
275	Nature of Cl bonding on the Au(111) surface: evidence of a mainly covalent interaction. *Journal of the American Chemical Society*, **2008**, 130, 3720-1	16.4	57
274	Determination of DNA-base orientation on carbon nanotubes through directional optical absorbance. *Nano Letters*, **2007**, 7, 2312-6	11.5	56
273	Contrasting growth modes of Mn on Ge(100) and Ge(111) surfaces: subsurface segregation versus intermixing. *Physical Review Letters*, **2004**, 93, 126102	7.4	56
272	Anatomy of the Photochemical Reaction: Excited-State Dynamics Reveals the C-H Acidity Mechanism of Methoxy Photo-oxidation on Titania. *Journal of Physical Chemistry Letters*, **2015**, 6, 1624-7	6.4	55
271	Long-Time Dynamics through Parallel Trajectory Splicing. *Journal of Chemical Theory and Computation*, **2016**, 12, 18-28	6.4	55
270	The Peierls-Nabarro model revisited. *Philosophical Magazine Letters*, **2000**, 80, 675-682	1	55

269	Structural model for a covalently bonded Si45 cluster. *Chemical Physics Letters*, **1989**, 163, 323-327	2.5	55
268	High-Temperature Quantum Anomalous Hall Effect in n-p Codoped Topological Insulators. *Physical Review Letters*, **2016**, 117, 056804	7.4	55
267	New classical potential for accurate simulation of atomic processes in Si. *Physical Review B*, **1988**, 38, 12736-12739	3.3	54
266	Stiffening of organosilicate glasses by organic cross-linking. *Acta Materialia*, **2011**, 59, 44-52	8.4	53
265	Role of chemical potentials in surface reconstruction: A new model and phase transition of GaAs(111)2x2. *Physical Review Letters*, **1986**, 56, 2819-2822	7.4	53
264	Quasiparticle band structures and interface physics of SnS and GeS. *Physical Review B*, **2013**, 87,	3.3	52
263	Hydrokinetic approach to large-scale cardiovascular blood flow. *Computer Physics Communications*, **2010**, 181, 462-472	4.2	52
262	Hyperon radiative decay. *Physical Review D*, **1985**, 32, 695-700	4.9	52
261	Energetics and Equilibrium Properties of Thin Pseudomorphic Si1□Cx(100) Layers in Si. *Physical Review Letters*, **1997**, 78, 3479-3482	7.4	51
260	Ground state of the strong-coupling Hubbard Hamiltonian: A numerical diagonalization study. *Physical Review B*, **1988**, 37, 656-659	3.3	51
259	Electronic-structure methods for twisted moir□layers. *Nature Reviews Materials*, **2020**, 5, 748-763	73.3	51
258	The chemical nature of surface point defects on MoO3(010): adsorption of hydrogen and methyl. *Journal of the American Chemical Society*, **2001**, 123, 2224-30	16.4	49
257	Implanted neural network potentials: Application to Li-Si alloys. *Physical Review B*, **2018**, 97,	3.3	48
256	Revealing the Empty-State Electronic Structure of Single-Unit-Cell FeSe/SrTiO3. *Physical Review Letters*, **2015**, 115, 017002	7.4	48
255	Selective thermal reduction of single-layer MoO3 nanostructures on Au(111). *Surface Science*, **2008**, 602, 1166-1174	1.8	48
254	Enhanced superconductivity upon weakening of charge density wave transport in 2H-TaS2 in the two-dimensional limit. *Physical Review B*, **2018**, 98,	3.3	46
253	Prediction of coronary artery plaque progression and potential rupture from 320-detector row prospectively ECG-gated single heart beat CT angiography: Lattice Boltzmann evaluation of endothelial shear stress. *International Journal of Cardiovascular Imaging*, **2009**, 25, 289-299	2.5	46
252	Nonorthogonal tight-binding Hamiltonians for defects and interfaces in silicon. *Physical Review B*, **1997**, 56, 10488-10496	3.3	46

251	Kinetic pathway for the formation of fe nanowires on stepped Cu111 surfaces. *Physical Review Letters*, **2005**, 94, 155503	7.4	45
250	Polarization switching in PbTiO3: an ab initio finite element simulation. *Acta Materialia*, **2002**, 50, 2989-3002	8.4	45
249	The nature of contact between Pd leads and semiconducting carbon nanotubes. *Nano Letters*, **2006**, 6, 1415-9	11.5	44
248	Variable stoichiometry surface reconstructions: New models for GaAs(1-bar1-bar1-bar) (2 x 2) and (sqrt 1-bar9-bar x sqrt 1-bar9-bar). *Physical Review Letters*, **1986**, 57, 106-109	7.4	44
247	Structural Properties of Defects in Glassy Liquids. *Journal of Physical Chemistry B*, **2016**, 120, 6139-46	3.4	44
246	Submonolayer island growth with adatom exchange. *Surface Science*, **1995**, 326, L483-L488	1.8	43
245	Interplay of Strain and Chemical Bonding in Surfactant Monolayers. *Europhysics Letters*, **1993**, 21, 685-690	1.6	43
244	Entropy calculation beyond the harmonic approximation: Application to diffusion by concerted exchange in Si. *Physical Review Letters*, **1991**, 66, 915-918	7.4	43
243	Topological flat bands in frustrated kagome lattice CoSn. *Nature Communications*, **2020**, 11, 4004	17.4	43
242	Strain effects on the behavior of isolated and paired sulfur vacancy defects in monolayer MoS2. *Physical Review B*, **2017**, 95,	3.3	42
241	Effects of alloying on the ductility of MoSi2single crystals from first-principles calculations. *Modelling and Simulation in Materials Science and Engineering*, **1998**, 6, 493-506	2	42
240	Real-Time TD-DFT with Classical Ion Dynamics: Methodology and Applications. *Journal of Chemical Theory and Computation*, **2016**, 12, 466-76	6.4	41
239	Nature of Oxidation of the Au(111) Surface: Experimental and Theoretical Investigation. *Journal of Physical Chemistry C*, **2009**, 113, 16561-16564	3.8	41
238	Kinetic energy density functionals for non-periodic systems. *Solid State Communications*, **2002**, 121, 281-286	2.6	41
237	Can vacancies lubricate dislocation motion in aluminum?. *Physical Review Letters*, **2002**, 89, 105501	7.4	41
236	Adsorption of As on stepped Si(100): Resolution of the sublattice-orientation dilemma. *Physical Review B*, **1991**, 44, 6534-6537	3.3	41
235	Theory of structural transformation in lithiated amorphous silicon. *Nano Letters*, **2014**, 14, 4065-70	11.5	40
234	Modeling Brittle and Ductile Behavior of Solids from First-Principles Calculations. *Physica Status Solidi (B): Basic Research*, **2000**, 217, 545-564	1.3	40

233	Multiple Epidemic Wave Model of the COVID-19 Pandemic: Modeling Study. *Journal of Medical Internet Research*, **2020**, 22, e20912	7.6	40
232	Morphological evolution of Si nanowires upon lithiation: a first-principles multiscale model. *Nano Letters*, **2013**, 13, 2011-5	11.5	39
231	D-π-A dye system containing cyano-benzoic acid as anchoring group for dye-sensitized solar cells. *Langmuir*, **2011**, 27, 14248-52	4	39
230	Graphene structures at an extreme degree of buckling. *ACS Nano*, **2011**, 5, 1395-400	16.7	39
229	Rich coordination chemistry of Au adatoms in gold sulfide monolayer on Au(111). *Journal of Physical Chemistry B*, **2006**, 110, 15663-5	3.4	39
228	Electronic structure of overstretched DNA. *Physical Review B*, **2002**, 66,	3.3	39
227	Adaptive coordinate, real-space electronic structure calculations on parallel computers. *Solid State Communications*, **1996**, 99, 57-61	1.6	39
226	(2 x 2) reconstructions of the {111} polar surfaces of GaAs. *Physical Review B*, **1986**, 33, 4406-4409	3.3	39
225	Mapping reactive flow patterns in monolithic nanoporous catalysts. *Microfluidics and Nanofluidics*, **2016**, 20, 1	2.8	38
224	Graphene hydrate: theoretical prediction of a new insulating form of graphene. *New Journal of Physics*, **2010**, 12, 125012	2.9	38
223	Electric-field control of magnetism in graphene quantum dots: Ab initio calculations. *Physical Review B*, **2010**, 82, 201411	3.3	38
222	Electronic structure theory of strained two-dimensional materials with hexagonal symmetry. *Physical Review B*, **2018**, 98,	3.3	37
221	New Pathway for Hot Electron Relaxation in Two-Dimensional Heterostructures. *Nano Letters*, **2018** , 18, 6057-6063	11.5	37
220	Mechanisms for ultrafast nonradiative relaxation in electronically excited eumelanin constituents. *Biophysical Journal*, **2008**, 95, 4396-402	2.9	37
219	Ultraheavy and Ultrarelativistic Dirac Quasiparticles in Sandwiched Graphenes. *Nano Letters*, **2020**, 20, 3030-3038	11.5	36
218	How Does Nanoporous Gold Dissociate Molecular Oxygen?. *Journal of Physical Chemistry C*, **2016**, 120, 16636-16640	3.8	36
217	Schottky barrier formation at a carbon nanotube–metal junction. *Applied Physics Letters*, **2006**, 89, 243107	3.4	36
216	Electronic states of group-IV endohedral atoms in C28. *Physical Review B*, **1993**, 48, 17556-17561	3.3	36

215	Noncovalent Bonding Controls Selectivity in Heterogeneous Catalysis: Coupling Reactions on Gold. *Journal of the American Chemical Society*, **2016**, 138, 15243-15250	16.4	35
214	HARES: an efficient method for first-principles electronic structure calculations of complex systems. *Computer Physics Communications*, **2001**, 137, 341-360	4.2	35
213	Thermodynamics of C incorporation on Si(100) from ab initio calculations. *Physical Review Letters*, **2001**, 86, 4556-9	7.4	35
212	Theory of electronic and optical properties of 3C-SiC. *Journal of Applied Physics*, **1999**, 85, 2179-2184	2.5	35
211	Atomic structure of surfactant monolayers and its role in epitaxial growth. *Materials Science and Engineering B: Solid-State Materials for Advanced Technology*, **1995**, 30, 175-186	3.1	35
210	Adatom diffusion by orchestrated exchange on semiconductor surfaces. *Physical Review Letters*, **1994**, 72, 1714-1717	7.4	35
209	Dry Dehydrogenation of Ethanol on PtCu Single Atom Alloys. *Topics in Catalysis*, **2018**, 61, 328-335	2.3	34
208	Establishing the limits of efficiency of perovskite solar cells from first principles modeling. *Scientific Reports*, **2016**, 6, 36108	4.9	34
207	Dilute Pd/Au Alloy Nanoparticles Embedded in Colloid-Templated Porous SiO2: Stable Au-Based Oxidation Catalysts. *Chemistry of Materials*, **2019**, 31, 5759-5768	9.6	34
206	Surface plasmon engineering in graphene functionalized with organic molecules: a multiscale theoretical investigation. *Nano Letters*, **2014**, 14, 50-6	11.5	34
205	Qualitative link between work of adhesion and thermal conductance of metal/diamond interfaces. *Journal of Applied Physics*, **2014**, 115, 123509	2.5	34
204	Structural role of RKS motifs in chromatin interactions: a molecular dynamics study of HP1 bound to a variably modified histone tail. *Biophysical Journal*, **2012**, 102, 1926-33	2.9	34
203	Effects of Knudsen diffusivity on the effective reactivity of nanoporous catalyst media. *Journal of Computational Science*, **2016**, 17, 377-383	3.4	34
202	Atomic electrostatic maps of 1D channels in 2D semiconductors using 4D scanning transmission electron microscopy. *Nature Communications*, **2019**, 10, 1127	17.4	33
201	Ab initio study of hydrogen adsorption on the Si(111)-(7 x 7) surface. *Physical Review B*, **1995**, 52, 17231-17237	3.5	33
200	New model for icosahedral carbon clusters and the structure of collapsed fullerite. *Physical Review Letters*, **1993**, 70, 2920-2923	7.4	33
199	Representations in neural network based empirical potentials. *Journal of Chemical Physics*, **2017**, 147, 024104	3.9	32
198	Ab initio determination of coarse-grained interactions in double-stranded DNA. *Journal of Chemical Physics*, **2012**, 137, 105102	3.9	32

197	Approaching the intrinsic band gap in suspended high-mobility graphene nanoribbons. *Physical Review B*, **2011**, 84,	3.3	32
196	Atomistic mechanisms for bilayer growth of graphene on metal substrates. *Physical Review B*, **2015**, 91,	3.3	30
195	Dynamics of the Photogenerated Hole at the Rutile TiO2(110)/Water Interface: A Nonadiabatic Simulation Study. *Journal of Physical Chemistry C*, **2014**, 118, 27393-27401	3.8	30
194	Direct imaging of atomic-scale ripples in few-layer graphene. *Nano Letters*, **2012**, 12, 2278-82	11.5	30
193	Theory of Adsorption and Desorption of H2 Molecules on the Si(111)- (7⁄7) surface. *Physical Review Letters*, **1997**, 79, 5078-5081	7.4	30
192	Slip energy barriers in aluminium and implications for ductile-brittle behaviour. *Philosophical Magazine A: Physics of Condensed Matter, Structure, Defects and Mechanical Properties*, **1997**, 75, 1117-1127		30
191	Tuning electronic properties of novel metal oxide nanocrystals using interface interactions: MoO3 monolayers on Au(1 1 1). *Surface Science*, **2005**, 577, L71-L77	1.8	30
190	Self-organized growth of Ge quantum dots on Si(001) substrates induced by sub-monolayer C coverages. *Nanotechnology*, **1999**, 10, 122-126	3.4	30
189	Microscopic model of heteroepitaxy of GaAs on Si(100). *Physical Review Letters*, **1989**, 62, 2484-2486	7.4	30
188	Theoretical investigation of the C60/copper phthalocyanine organic photovoltaic heterojunction. *Nano Research*, **2012**, 5, 248-257	10	29
187	Performance Analysis of the Lattice Boltzmann Model Beyond Navier-Stokes **2013**,		29
186	Quantized current blockade and hydrodynamic correlations in biopolymer translocation through nanopores: evidence from multiscale simulations. *Nano Letters*, **2008**, 8, 1115-9	11.5	29
185	Energetics of Ordered Structures in Molecular Hydrogen. *Europhysics Letters*, **1992**, 17, 151-155	1.6	29
184	Twisted Trilayer Graphene: A Precisely Tunable Platform for Correlated Electrons. *Physical Review Letters*, **2020**, 125, 116404	7.4	29
183	Lithium Intercalation in Graphene⁄MoS2 Heterostructures. *Journal of Physical Chemistry C*, **2018**, 122, 24535-24541	3.8	29
182	Dumbbell Defects in FeSe Films: A Scanning Tunneling Microscopy and First-Principles Investigation. *Nano Letters*, **2016**, 16, 4224-9	11.5	28
181	Optical and elastic properties of diamond-like carbon with metallic inclusions: A theoretical study. *Journal of Applied Physics*, **2012**, 112, 103503	2.5	28
180	Symmetry and stability of solitary dimer rows on Si(100). *Physical Review Letters*, **1993**, 70, 2589-2592	7.4	28

179	Electronic properties of a cluster-based solid form of carbon: C28 hyperdiamond. *Physical Review B*, **1994**, 49, 8446-8453	3.3	28
178	Li intercalation at graphene/hexagonal boron nitride interfaces. *Physical Review B*, **2016**, 93,	3.3	27
177	Structural, electronic, and optical properties of representative Cu-flavonoid complexes. *Journal of Physical Chemistry B*, **2009**, 113, 6478-83	3.4	27
176	Electronic nature of step-edge barriers against adatom descent on transition-metal surfaces. *Physical Review Letters*, **2008**, 101, 216101	7.4	27
175	Electric field tuning of oxygen stoichiometry at oxide surfaces: molecular dynamics simulations studies of zirconia. *Energy and Environmental Science*, **2009**, 2, 1196	35.4	26
174	Derivation of Wannier orbitals and minimal-basis tight-binding Hamiltonians for twisted bilayer graphene: First-principles approach. *Physical Review Research*, **2019**, 1,	3.9	26
173	Effective Hamiltonian for FeAs-based superconductors. *Physical Review B*, **2008**, 78,	3.3	25
172	Formation of monatomic Fe chains on vicinal Cu(111) surfaces: An atomistic view. *Physical Review B*, **2006**, 73,	3.3	25
171	In situ nanoscale imaging of moir□superlattices in twisted van der Waals heterostructures. *Nature Communications*, **2020**, 11, 4209	17.4	25
170	Review of atomistic simulations of surface diffusion and growth on semiconductors. *Computational Materials Science*, **1996**, 6, 158-172	3.2	24
169	Atomistic aspects of diffusion and growth on the Si and Ge (111) surfaces. *Thin Solid Films*, **1996**, 272, 386-398	2.2	24
168	Contribution of concerted exchange to the entropy of self-diffusion in Si. *Physical Review B*, **1993**, 47, 1659-1662	3.3	24
167	Epsilon-near-zero behavior from plasmonic Dirac point: Theory and realization using two-dimensional materials. *Physical Review B*, **2016**, 94,	3.3	23
166	Structural stability and electronic properties of low-index surfaces of SnS. *Journal of Applied Physics* , **2014**, 115, 173702	2.5	23
165	Multiscale Simulation of Cardiovascular flows on the IBM Bluegene/P: Full Heart-Circulation System at Red-Blood Cell Resolution **2010**,		23
164	Enhancement of van der Waals Interlayer Coupling through Polar Janus MoSSe. *Journal of the American Chemical Society*, **2020**, 142, 17499-17507	16.4	23
163	Dihedral-angle-corrected registry-dependent interlayer potential for multilayer graphene structures. *Physical Review B*, **2018**, 98,	3.3	23
162	Accurate formation energies of charged defects in solids: A systematic approach. *Physical Review B*, **2017**, 95,	3.3	22

161	Chlorine interaction with defects on the Au(111) surface: a first-principles theoretical investigation. *Journal of Chemical Physics*, **2008**, 129, 104702	3.9	22
160	Substitutional carbon impurities in thin silicon films: Equilibrium structure and properties. *Journal of Vacuum Science & Technology an Official Journal of the American Vacuum Society B, Microelectronics Processing and Phenomena*, **1998**, 16, 1687		22
159	The first 100 days: Modeling the evolution of the COVID-19 pandemic. *Chaos, Solitons and Fractals*, **2020**, 138, 110114	9.3	22
158	Direct visualization of quasi-ordered oxygen chain structures on Au(110)-(1 □2). *Surface Science*, **2016**, 650, 5-10	1.8	22
157	Moir□metrology of energy landscapes in van der Waals heterostructures. *Nature Communications*, **2021**, 12, 242	17.4	22
156	Orientational order in dense molecular hydrogen: A first-principles path-integral Monte Carlo calculation. *Physical Review B*, **1994**, 49, 11822-11832	3.3	21
155	Theoretical study of passivated small fullerenes C24X4 (X?N, P, As) and their isoelectronic equivalents (BN)12X4. *Chemical Physics Letters*, **1994**, 225, 448-453	2.5	21
154	Clean 2D superconductivity in a bulk van der Waals superlattice. *Science*, **2020**, 370, 231-236	33.3	21
153	Effect of nanoscale flows on the surface structure of nanoporous catalysts. *Journal of Chemical Physics*, **2017**, 146, 214703	3.9	20
152	Lattice Boltzmann Simulation of Reactive Microflows over Catalytic Surfaces. *Journal of Statistical Physics*, **2002**, 107, 343-366	1.5	20
151	Finite-temperature molecular-dynamics study of unstable stacking fault free energies in silicon. *Physical Review B*, **1998**, 58, 12555-12558	3.3	20
150	Development of robust neural-network interatomic potential for molten salt. *Cell Reports Physical Science*, **2021**, 2, 100359	6.1	20
149	Energetics and kinetics of vacancy defects in 4H-SiC. *Physical Review B*, **2018**, 98,	3.3	20
148	Polyiodide-Doped Graphene. *Journal of Physical Chemistry C*, **2017**, 121, 609-615	3.8	19
147	Machine Learning Prediction of H Adsorption Energies on Ag Alloys. *Journal of Chemical Information and Modeling*, **2019**, 59, 1357-1365	6.1	19
146	Multiscale Simulation of Nanobiological Flows. *Computing in Science and Engineering*, **2008**, 10, 10-19	1.5	19
145	Energetics of large lattice strains: Application to silicon. *Physical Review B*, **1994**, 50, 1535-1540	3.3	19
144	Evolution of steady-state material properties during catalysis: Oxidative coupling of methanol over nanoporous Ag0.03Au0.97. *Journal of Catalysis*, **2019**, 380, 366-374	7.3	18

143	Structure of incommensurate gold sulfide monolayer on Au(111). *Journal of Chemical Physics*, **2007**, 127, 104704	3.9	18
142	Superconducting and charge□density wave instabilities in ultrasmall-radius carbon nanotubes. *Solid State Communications*, **2005**, 135, 335-339	1.6	18
141	Linking chemical reactivity, magic numbers, and local electronic properties of clusters. *Physical Review B*, **1999**, 59, 7745-7750	3.3	18
140	Creating Weyl nodes and controlling their energy by magnetization rotation. *Physical Review Research*, **2019**, 1,	3.9	18
139	Electric field tuning of band offsets in transition metal dichalcogenides. *Physical Review B*, **2016**, 94,	3.3	18
138	Perturbation theory for weakly coupled two-dimensional layers. *Journal of Materials Research*, **2016** , 31, 959-966	2.5	18
137	Simultaneous Identification of Low and High Atomic Number Atoms in Monolayer 2D Materials Using 4D Scanning Transmission Electron Microscopy. *Nano Letters*, **2019**, 19, 6482-6491	11.5	17
136	Surface-reconstruction-induced geometries of Si clusters. *Physical Review B*, **1997**, 56, 13455-13463	3.3	17
135	Water wettability of close-packed metal surfaces. *Journal of Chemical Physics*, **2007**, 127, 244710	3.9	17
134	Density-functional theory modeling of bulk magnetism with spin-dependent pseudopotentials. *Physical Review B*, **2001**, 64,	3.3	17
133	Macroscopic 3D Nanoporosity Formation by Dry Oxidation of AgAu Alloys. *Journal of Physical Chemistry C*, **2017**, 121, 5115-5122	3.8	16
132	Surfactant-Mediated Growth and Patterning of Atomically Thin Transition Metal Dichalcogenides. *ACS Nano*, **2020**, 14, 6570-6581	16.7	16
131	Resolving discrepancies between LEED and STM through ab initio calculations: Surface and bonding of sulfur on Mo(110). *Physical Review B*, **1999**, 60, 11783-11788	3.3	16
130	Scanning tunneling microscopy and first-principles theory of the Sn/GaAs(110) surface. *Physical Review B*, **1989**, 40, 10044-10047	3.3	16
129	Twofold van Hove singularity and origin of charge order in topological kagome superconductor CsV3Sb5. *Nature Physics*,	16.2	16
128	Electronic structure calculations of twisted multi-layer graphene superlattices. *2D Materials*, **2020**, 7, 035028	5.9	15
127	General Effect of van der Waals Interactions on the Stability of Alkoxy Intermediates on Metal Surfaces. *Journal of Physical Chemistry B*, **2018**, 122, 555-560	3.4	15
126	Controlling O coverage and stability by alloying Au and Ag. *Physical Chemistry Chemical Physics*, **2016**, 18, 26844-26853	3.6	15

125	Nanoribbon edges of transition-metal dichalcogenides: Stability and electronic properties. *Physical Review B*, **2017**, 96,	3.3	15
124	Role of defects in propene adsorption and reaction on a partially O-covered Au(111) surface. *Catalysis Science and Technology*, **2011**, 1, 1166	5.5	15
123	Insights from Theory on the Relationship Between Surface Reactivity and Gold Atom Release. *Topics in Catalysis*, **2010**, 53, 365-377	2.3	15
122	Active role of buried ultrathin oxide layers in adsorption of O2 on Au films. *Surface Science*, **2006**, 600, 3388-3393	1.8	14
121	Variational finite-difference representation of the kinetic energy operator. *Physical Review B*, **2001**, 64,	3.3	14
120	<331> slip on {013} planes in molybdenum disilicide. *Philosophical Magazine A: Physics of Condensed Matter, Structure, Defects and Mechanical Properties*, **1999**, 79, 655-663		14
119	Structural models for intermediate-sized Si clusters. *Zeitschrift Fü Physik D-Atoms Molecules and Clusters*, **1993**, 26, 346-348		14
118	On the possibility of two-dimensional growth of GaAs on atomically flat Si(100) surfaces. *Surface Science*, **1989**, 224, 515-524	1.8	14
117	Water facilitates oxygen migration on gold surfaces. *Physical Chemistry Chemical Physics*, **2018**, 20, 2196-2204	3.3	14
116	Modeling mechanical relaxation in incommensurate trilayer van der Waals heterostructures. *Physical Review B*, **2020**, 101,	3.3	13
115	Catalyst design for enhanced sustainability through fundamental surface chemistry. *Philosophical Transactions Series A, Mathematical, Physical, and Engineering Sciences*, **2016**, 374,	3	13
114	Multiscale Hemodynamics Using GPU Clusters. *Communications in Computational Physics*, **2012**, 11, 48-64	2.4	13
113	Local Bonding Effects in the Oxidation of CO on Oxygen-Covered Au(111) from Ab Initio Molecular Dynamics Simulations. *Journal of Chemical Theory and Computation*, **2010**, 6, 279-87	6.4	13
112	Compositional tuning of ultrathin surface oxides on metal and alloy substrates using photons: Dynamic simulations and experiments. *Physical Review B*, **2010**, 81,	3.3	13
111	EXPLORING DNA TRANSLOCATION THROUGH A NANOPORE VIA A MULTISCALE LATTICE-BOLTZMANN MOLECULAR-DYNAMICS METHODOLOGY. *International Journal of Modern Physics C*, **2007**, 18, 685-692	1.1	13
110	Quantum plasmons with optical-range frequencies in doped few-layer graphene. *Physical Review B*, **2018**, 97,	3.3	13
109	A Comparative Ab Initio Study of Anhydrous Dehydrogenation of Linear-Chain Alcohols on Cu(110). *Journal of Physical Chemistry C*, **2018**, 122, 7806-7815	3.8	12
108	Optical properties of clusters and molecules from real-time time-dependent density functional theory using a self-consistent field. *Molecular Physics*, **2010**, 108, 1829-1844	1.7	12

107	Dinitrosyl formation as an intermediate stage of the reduction of NO in the presence of MoO3. *Journal of Chemical Physics*, **2003**, 118, 6046-6051	3.9	12
106	Free energy of the concerted-exchange mechanism for self-diffusion in silicon. *Physical Review B*, **1996**, 53, 1310-1314	3.3	12
105	Exploring the structure of solids through magic strains: prediction of a new metallic phase of Si. *Modelling and Simulation in Materials Science and Engineering*, **1992**, 1, 91-100	2	12
104	Localized adatom vibrations in Si clusters. *Physical Review B*, **1991**, 44, 8334-8337	3.3	12
103	Anhydrous Methanol and Ethanol Dehydrogenation at Cu(111) Step Edges. *Journal of Physical Chemistry C*, **2018**, 122, 21952-21962	3.8	12
102	Dual role of Fe dopants in enhancing stability and charge transfer in (Li0.8Fe0.2)OHFeSe superconductors. *Physical Review B*, **2016**, 93,	3.3	11
101	Bounds on nanoscale nematicity in single-layer FeSe/SrTiO3. *Physical Review B*, **2016**, 93,	3.3	11
100	A force-matching Stillinger-Weber potential for MoS2: Parameterization and Fisher information theory based sensitivity analysis. *Journal of Applied Physics*, **2017**, 122, 244301	2.5	11
99	Orbital-free density functional theory applied to NaAlH4. *Journal of Physical Chemistry B*, **2005**, 109, 16554-62	3.4	11
98	Theory of spintronic materials. *Physica Status Solidi (B): Basic Research*, **2006**, 243, 2133-2150	1.3	11
97	First-principles studies of the electronic structure of cyclopentene on Si(001): density functional theory and GW calculations. *Physica Status Solidi (B): Basic Research*, **2006**, 243, 2048-2053	1.3	11
96	Electronic and optical properties of Si1−yCy alloys. *Physical Review B*, **1999**, 60, 11494-11502	3.3	11
95	Variational Hilbert-space-truncation approach to quantum Heisenberg antiferromagnets on frustrated clusters. *Physical Review B*, **1996**, 53, 2546-2555	3.3	11
94	Isolated As antisite in GaAs: Possibility of the EL2 defect. *Physical Review B*, **1989**, 40, 8020-8023	3.3	11
93	Monolayer Honeycomb Borophene: A Promising Anode Material with a Record Capacity for Lithium-Ion and Sodium-Ion Batteries. *Journal of the Electrochemical Society*, **2020**, 167, 090527	3.9	11
92	Data-driven studies of magnetic two-dimensional materials. *Scientific Reports*, **2020**, 10, 15795	4.9	10
91	Effects of lithium intercalation in twisted bilayer graphene. *Physical Review B*, **2020**, 101,	3.3	9
90	Identifying key descriptors in surface binding: interplay of surface anchoring and intermolecular interactions for carboxylates on Au(110). *Chemical Science*, **2018**, 9, 3759-3766	9.4	9

89	A lattice Boltzmann study of reactive microflows. *Computer Physics Communications*, **2002**, 147, 516-521	4.2	9
88	A density functional theory study of site-specific methyl reaction on MoO3(010): The effects of methyl coverage. *Journal of Chemical Physics*, **2000**, 112, 9617-9623	3.9	9
87	Metal-coated fullerenes: electronic, geometrical and vibrational properties of C60M62 (M=Ti and V). *Chemical Physics Letters*, **1999**, 303, 373-378	2.5	9
86	Theoretical study of cubic structures based on fullerene carbon clusters: C28C and (C28)2. *Physical Review B*, **1995**, 52, 2125-2130	3.3	9
85	Theory of surfactant-mediated growth on semiconductor surfaces. *Applied Surface Science*, **1996**, 102, 3-5	6.7	9
84	Effect of Frustrated Rotations on the Pre-Exponential Factor for Unimolecular Reactions on Surfaces: A Case Study of Alkoxy Dehydrogenation. *Journal of Physical Chemistry C*, **2020**, 124, 1429-1437	3.8	9
83	Parallel in time approximation of the lattice Boltzmann method for laminar flows. *Journal of Computational Physics*, **2014**, 270, 577-586	4.1	8
82	Quantum phase transitions and topological proximity effects in graphene nanoribbon heterostructures. *Nanoscale*, **2014**, 6, 3259-67	7.7	8
81	First-principles study of static nanoscale friction between MoO3 and MoS2. *Journal of Computer-Aided Materials Design*, **1998**, 5, 61-71		8
80	Compact carbon clusters with tetrahedral bonding and icosahedral symmetry. *Computational Materials Science*, **1993**, 1, 403-410	3.2	8
79	Orderly disorder in magic-angle twisted trilayer graphene.. *Science*, **2022**, 376, 193-199	33.3	8
78	Robust prediction of complex spatiotemporal states through machine learning with sparse sensing. *Physics Letters, Section A: General, Atomic and Solid State Physics*, **2020**, 384, 126300	2.3	7
77	Nonadiabatic Hydrogen Dissociation on Copper Nanoclusters. *Journal of Physical Chemistry Letters*, **2018**, 9, 5339-5343	6.4	7
76	Is the nature of magnetic order in copper-oxides and in iron-pnictides different?. *Solid State Communications*, **2010**, 150, 62-65	1.6	7
75	Embedded atom method potentials employing a faithful density representation. *Modelling and Simulation in Materials Science and Engineering*, **2006**, 14, 721-731	2	7
74	Duality between atomic configurations and Bloch states in twistronic materials. *Physical Review Research*, **2020**, 2,	3.9	7
73	The effect of Ag, Pb and Bi impurities on grain boundary sliding and intergranular decohesion in Copper. *Philosophical Magazine*, **2016**, 96, 2868-2886	1.6	7
72	Observation of interband collective excitations in twisted bilayer graphene. *Nature Physics*,	16.2	7

71	Identification of defects at the interface between 3C-SiC quantum dots and a SiO2 embedding matrix. *Physica Status Solidi (B): Basic Research*, **2012**, 249, 360-367	1.3	6
70	Interatomic Potential for Condensed Phases and Bulk Defects in Silicon. *Materials Research Society Symposia Proceedings*, **1997**, 469, 217		6
69	Electronic structure of Pd-covered (10,0) carbon nanotube. *Physica Status Solidi (B): Basic Research*, **2006**, 243, 2164-2169	1.3	6
68	Spectroscopic Signatures of Interlayer Coupling in Janus MoSSe/MoS Heterostructures. *ACS Nano*, **2021**, 15, 14394-14403	16.7	6
67	Imaginary-Time Time-Dependent Density Functional Theory and Its Application for Robust Convergence of Electronic States. *Journal of Chemical Theory and Computation*, **2019**, 15, 6036-6045	6.4	5
66	Numerical simulation of conformational variability in biopolymer translocation through wide nanopores. *Journal of Statistical Mechanics: Theory and Experiment*, **2009**, 2009, P06009	1.9	5
65	The Environment-Dependent Interatomic Potential Applied To Silicon Disordered Structures And Phase Transitions. *Materials Research Society Symposia Proceedings*, **1997**, 491, 339		5
64	Semiconducting cyanide-transition-metal nanotubes. *Small*, **2007**, 3, 1253-8	11	5
63	Multiscale model of electronic behavior and localization in stretched dry DNA. *Journal of Materials Science*, **2007**, 42, 8894-8903	4.3	5
62	Modeling of the carbon-rich c(4□) reconstruction on Si(100). *Surface Science*, **2004**, 554, 90-102	1.8	5
61	Theory of the (3□) reconstruction of the GaAs(001) surface. *Materials Science and Engineering B: Solid-State Materials for Advanced Technology*, **1999**, 67, 1-6	3.1	5
60	Low-cost visible-light photosynthesis of water and adsorbed carbon dioxide into long-chain hydrocarbons. *Chemical Physics Letters*, **2020**, 739, 136985	2.5	5
59	How carbon vacancies can affect the properties of group IV color centers in diamond: A study of thermodynamics and kinetics. *Journal of Applied Physics*, **2019**, 126, 195103	2.5	5
58	Evidence of two-dimensional flat band at the surface of antiferromagnetic kagome metal FeSn. *Nature Communications*, **2021**, 12, 5345	17.4	5
57	A Self-Consistent Charge Density-Functional Based Tight-Binding Scheme for Large Biomolecules **2000**, 217, 357		5
56	Interaction of DNA with CNTs: Properties and Prospects for Electronic Sequencing67-96		4
55	Multiscale simulations of complex systems: computation meets reality. *Scientific Modeling and Simulation SMNS*, **2008**, 15, 59-65		4
54	High-pressure plastic flow in silicon: A first-principles theoretical study. *Journal of Computer-Aided Materials Design*, **1993**, 1, 55-62		4

53	Correlated Insulating States and Transport Signature of Superconductivity in Twisted Trilayer Graphene Superlattices. *Physical Review Letters*, **2021**, 127, 166802	7.4	4
52	Geometric origins of topological insulation in twisted layered semiconductors. *Physical Review B*, **2021**, 104,	3.3	4
51	Lithium intercalation in MoS2 bilayers and implications for moir flat bands. *Physical Review B*, **2020**, 102,	3.3	4
50	Imprinting Tunable Magnetism in Graphene Nanoribbons via Edge Extensions. *Journal of Physical Chemistry Letters*, **2021**, 12, 1214-1219	6.4	4
49	Reaction-Induced Excitations and Their Effect on Surface Chemistry. *ACS Catalysis*, **2018**, 8, 10358-10363	13.1	4
48	First-principles study of coupled effect of ripplocations and S-vacancies in MoS2. *Journal of Applied Physics*, **2019**, 126, 084303	2.5	3
47	Universal behavior of a dispersive Dirac cone in gradient-index plasmonic metamaterials. *Physical Review B*, **2018**, 97,	3.3	3
46	Structure and Properties of Covalently Bonded Si Clusters. *Materials Science Forum*, **1996**, 232, 67-86	0.4	3
45	Shape of Small Silicon Clusters. *Physical Review Letters*, **1993**, 71, 2354-2354	7.4	3
44	Thermodynamic and kinetic aspects of GaAs growth on Si(100). *Superlattices and Microstructures*, **1990**, 8, 229-232	2.8	3
43	Boosting the efficiency of ab initio electron-phonon coupling calculations through dual interpolation. *Physical Review B*, **2020**, 102,	3.3	3
42	Density functional theory beyond the Born-Oppenheimer approximation: Accurate treatment of the ionic zero-point motion. *Physical Review B*, **2018**, 98,	3.3	3
41	Emergence and dynamical properties of stochastic branching in the electronic flows of disordered Dirac solids. *Europhysics Letters*, **2018**, 122, 27003	1.6	3
40	LAN: A Materials Notation for Two-Dimensional Layered Assemblies. *Journal of Chemical Information and Modeling*, **2020**, 60, 3457-3462	6.1	2
39	Compression of Wannier functions into Gaussian-type orbitals. *Computer Physics Communications*, **2018**, 230, 27-37	4.2	2
38	Bottom-up Modeling of the Elastic Properties of Organosilicate Glasses and their Relation to Composition and Network Defects. *Materials Research Society Symposia Proceedings*, **2011**, 1297, 17		2
37	Annealing simulations to determine the matrix interface structure of SiC quantum dots embedded in SiO2. *Physica Status Solidi C: Current Topics in Solid State Physics*, **2010**, 7, 407-410		2
36	MUPHY: A parallel high performance MUlti PHYsics/Scale code. *Parallel and Distributed Processing Symposium (IPDPS), Proceedings of the International Conference on*, **2008**,		2

35	A Self-Consistent Charge Density-Functional Based Tight-Binding Scheme for Large Biomolecules **2005**, 357-376		2
34	Derivation of Interatomic Potentials by Inversion of Ab Initio Cohesive Energy Curves. *Materials Research Society Symposia Proceedings*, **1995**, 408, 79		2
33	Kaxiras replies. *Physical Review Letters*, **1991**, 66, 2687	7.4	2
32	Theoretical modeling of heteroepitaxial growth initiation. *Materials Science and Engineering B: Solid-State Materials for Advanced Technology*, **1992**, 14, 245-253	3.1	2
31	Modeling the effect of the vaccination campaign on the Covid-19 pandemic. *Chaos, Solitons and Fractals*, **2021**, 154, 111621	9.3	2
30	Role of Explicitly Included Solvents on Ultrafast Electron Injection and Recombination Dynamics at TiO/Dye Interfaces. *ACS Applied Materials & Interfaces*, **2020**, 12, 49174-49181	9.5	2
29	Nonadiabatic dynamics of cobalt tricarbonyl nitrosyl for ligand dissociation induced by electronic excitation. *Scientific Reports*, **2021**, 11, 8997	4.9	2
28	Progressive Phosphorylation Modulates the Self-Association of a Variably Modified Histone H3 Peptide. *Frontiers in Molecular Biosciences*, **2021**, 8, 698182	5.6	2
27	Homogenization of plasmonic crystals: seeking the epsilon-near-zero effect. *Proceedings of the Royal Society A: Mathematical, Physical and Engineering Sciences*, **2019**, 475, 20190220	2.4	2
26	Calculating the hyperfine tensors for group-IV impurity-vacancy centers in diamond using hybrid density functional theory. *Physical Review B*, **2021**, 104,	3.3	2
25	Microscopic origin of the high thermoelectric figure of merit of n-doped SnSe. *Physical Review B*, **2021**, 104,	3.3	2
24	Modeling Brittle and Ductile Behavior of Solids from First-Principles Calculations **2000**, 217, 545		2
23	Impact of Vibrations and Electronic Coherence on Electron Transfer in Flat Molecular Wires. *MRS Advances*, **2017**, 2, 811-816	0.7	1
22	High Resolution Sculpting and Imaging for Graphene Nano-structures. *Microscopy and Microanalysis* , **2009**, 15, 1166-1167	0.5	1
21	Dynamic scaling in conserved systems with coupled fields: Application to surfactant-mediated growth. *Europhysics Letters*, **1996**, 36, 129-134	1.6	1
20	Crystalline Structure Around the Single Vacancy in Silicon: Formation Volume and Stress Effects. *Materials Research Society Symposia Proceedings*, **1998**, 527, 377		1
19	Electronic states and charge-transfer mechanisms in solid molecular hydrogen. *Computational Materials Science*, **1995**, 3, 368-376	3.2	1
18	Electrically Induced Dirac Fermions in Graphene Nanoribbons. *Nano Letters*, **2021**, 21, 9332-9338	11.5	1

17	Effects of structural distortions on the electronic structure of T-type transition metal dichalcogenides. *Physical Review B*, **2020**, 102,	3.3	1
16	A Self-Consistent Charge Density-Functional Based Tight-Binding Scheme for Large Biomolecules **2000**, 217, 357		1
15	Signatures of bosonic Landau levels in a finite-momentum superconductor. *Nature*, **2021**, 599, 51-56	50.4	0
14	Theoretical investigation of charge transfer between the NV center in diamond and substitutional N and P. *Journal of Applied Physics*, **2021**, 130, 155102	2.5	0
13	Group theoretical analysis of nitrogen-vacancy centers energy levels and selection rules. *Materials Research Society Symposia Proceedings*, **2011**, 1282, 95		
12	Topological Graphene Imaging and Fabrication of Devices. *Microscopy and Microanalysis*, **2012**, 18, 1534-1535	0.5	
11	Ab-Initio Theory of Initial Oxidation of Silicon (001) Surfaces. *Materials Research Society Symposia Proceedings*, **1997**, 492, 189		
10	Atomistic features of the amorphous crystal interface in silicon. *Journal of Computer-Aided Materials Design*, **1998**, 5, 55-60		
9	Modeling Brittle and Ductile Behavior of Solids from First-Principles Calculations **2005**, 545-564		
8	Ab-Initio Studies of AlSb (001) Adatom Behavior and Reconstruction. *Materials Research Society Symposia Proceedings*, **2000**, 618, 11		
7	Crystalline Structure Around the Single Vacancy in Silicon: Formation Volume and Stress Effects. *Materials Research Society Symposia Proceedings*, **1998**, 532, 199		
6	First-Principles Study of SI(lll) Homoepitaxy. *Materials Research Society Symposia Proceedings*, **1998**, 538, 341		
5	Unstable Stacking Fault Free Energies in Silicon through Empirical Modeling. *Materials Research Society Symposia Proceedings*, **1998**, 539, 175		
4	Simulations of structural materials. *Journal of Computer-Aided Materials Design*, **1996**, 3, 30-35		
3	O(N) Scaling Simulations of Silicon Bulk and Surface Properties Based on a Non-Orthogonal Tight-Binding Hamiltonian. *Materials Research Society Symposia Proceedings*, **1995**, 408, 55		
2	Acres: Adaptive Coordinate Real-Space Electronic Structure. *Materials Research Society Symposia Proceedings*, **1995**, 408, 139		
1	Reply to "Comment on 'Ground state of the strong-coupling Hubbard Hamiltonian: A numerical diagonalization study' ". *Physical Review B*, **1989**, 40, 2596-2597	3.3	