Efthimios Kaxiras

List of Publications by Year in Descending Order

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	Orderly disorder in magic-angle twisted trilayer graphene.. *Science*, **2022**, 376, 193-199	33.3	8
393	Signatures of bosonic Landau levels in a finite-momentum superconductor. *Nature*, **2021**, 599, 51-56	50.4	0
392	Modeling the effect of the vaccination campaign on the Covid-19 pandemic. *Chaos, Solitons and Fractals*, **2021**, 154, 111621	9.3	2
391	Correlated Insulating States and Transport Signature of Superconductivity in Twisted Trilayer Graphene Superlattices. *Physical Review Letters*, **2021**, 127, 166802	7.4	4
390	Geometric origins of topological insulation in twisted layered semiconductors. *Physical Review B*, **2021**, 104,	3.3	4
389	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
388	Electrically Induced Dirac Fermions in Graphene Nanoribbons. *Nano Letters*, **2021**, 21, 9332-9338	11.5	1
387	Development of robust neural-network interatomic potential for molten salt. *Cell Reports Physical Science*, **2021**, 2, 100359	6.1	20
386	Nonadiabatic dynamics of cobalt tricarbonyl nitrosyl for ligand dissociation induced by electronic excitation. *Scientific Reports*, **2021**, 11, 8997	4.9	2
385	Progressive Phosphorylation Modulates the Self-Association of a Variably Modified Histone H3 Peptide. *Frontiers in Molecular Biosciences*, **2021**, 8, 698182	5.6	2
384	Moir□metrology of energy landscapes in van der Waals heterostructures. *Nature Communications*, **2021**, 12, 242	17.4	22
383	Imprinting Tunable □Magnetism in Graphene Nanoribbons via Edge Extensions. *Journal of Physical Chemistry Letters*, **2021**, 12, 1214-1219	6.4	4
382	Spectroscopic Signatures of Interlayer Coupling in Janus MoSSe/MoS Heterostructures. *ACS Nano*, **2021**, 15, 14394-14403	16.7	6
381	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
380	Microscopic origin of the high thermoelectric figure of merit of n-doped SnSe. *Physical Review B*, **2021**, 104,	3.3	2
379	Evidence of two-dimensional flat band at the surface of antiferromagnetic kagome metal FeSn. *Nature Communications*, **2021**, 12, 5345	17.4	5
378	Electronic structure calculations of twisted multi-layer graphene superlattices. *2D Materials*, **2020**, 7, 035028	5.9	15

377	LAN: A Materials Notation for Two-Dimensional Layered Assemblies. *Journal of Chemical Information and Modeling*, **2020**, 60, 3457-3462	6.1	2
376	Modeling mechanical relaxation in incommensurate trilayer van der Waals heterostructures. *Physical Review B*, **2020**, 101,	3.3	13
375	Ultraheavy and Ultrarelativistic Dirac Quasiparticles in Sandwiched Graphenes. *Nano Letters*, **2020**, 20, 3030-3038	11.5	36
374	Effects of lithium intercalation in twisted bilayer graphene. *Physical Review B*, **2020**, 101,	3.3	9
373	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
372	Surfactant-Mediated Growth and Patterning of Atomically Thin Transition Metal Dichalcogenides. *ACS Nano*, **2020**, 14, 6570-6581	16.7	16
371	Duality between atomic configurations and Bloch states in twistronic materials. *Physical Review Research*, **2020**, 2,	3.9	7
370	Multiple Epidemic Wave Model of the COVID-19 Pandemic: Modeling Study. *Journal of Medical Internet Research*, **2020**, 22, e20912	7.6	40
369	Data-driven studies of magnetic two-dimensional materials. *Scientific Reports*, **2020**, 10, 15795	4.9	10
368	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
367	Dirac fermions and flat bands in the ideal kagome metal FeSn. *Nature Materials*, **2020**, 19, 163-169	27	121
366	Low-cost visible-light photosynthesis of water and adsorbed carbon dioxide into long-chain hydrocarbons. *Chemical Physics Letters*, **2020**, 739, 136985	2.5	5
365	Clean 2D superconductivity in a bulk van der Waals superlattice. *Science*, **2020**, 370, 231-236	33.3	21
364	Effects of structural distortions on the electronic structure of T-type transition metal dichalcogenides. *Physical Review B*, **2020**, 102,	3.3	1
363	The first 100 days: Modeling the evolution of the COVID-19 pandemic. *Chaos, Solitons and Fractals*, **2020**, 138, 110114	9.3	22
362	Topological flat bands in frustrated kagome lattice CoSn. *Nature Communications*, **2020**, 11, 4004	17.4	43
361	Electronic-structure methods for twisted moir layers. *Nature Reviews Materials*, **2020**, 5, 748-763	73.3	51
360	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

359	Enhancement of van der Waals Interlayer Coupling through Polar Janus MoSSe. *Journal of the American Chemical Society*, **2020**, 142, 17499-17507	16.4	23
358	Lithium intercalation in MoS2 bilayers and implications for moiré flat bands. *Physical Review B*, **2020**, 102,	3.3	4
357	Boosting the efficiency of ab initio electron-phonon coupling calculations through dual interpolation. *Physical Review B*, **2020**, 102,	3.3	3
356	Twisted Trilayer Graphene: A Precisely Tunable Platform for Correlated Electrons. *Physical Review Letters*, **2020**, 125, 116404	7.4	29
355	In situ nanoscale imaging of moiré superlattices in twisted van der Waals heterostructures. *Nature Communications*, **2020**, 11, 4209	17.4	25
354	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
353	First-principles study of coupled effect of ripplocations and S-vacancies in MoS2. *Journal of Applied Physics*, **2019**, 126, 084303	2.5	3
352	Enhancement of interlayer exchange in an ultrathin two-dimensional magnet. *Nature Physics*, **2019**, 15, 1255-1260	16.2	85
351	Atomic and electronic reconstruction at the van der Waals interface in twisted bilayer graphene. *Nature Materials*, **2019**, 18, 448-453	27	282
350	Machine Learning Prediction of H Adsorption Energies on Ag Alloys. *Journal of Chemical Information and Modeling*, **2019**, 59, 1357-1365	6.1	19
349	Atomic electrostatic maps of 1D channels in 2D semiconductors using 4D scanning transmission electron microscopy. *Nature Communications*, **2019**, 10, 1127	17.4	33
348	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
347	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
346	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
345	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
344	Exact continuum model for low-energy electronic states of twisted bilayer graphene. *Physical Review Research*, **2019**, 1,	3.9	105
343	Creating Weyl nodes and controlling their energy by magnetization rotation. *Physical Review Research*, **2019**, 1,	3.9	18
342	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

341	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
340	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
339	Observation of the nonlinear Hall effect under time-reversal-symmetric conditions. *Nature*, **2019**, 565, 337-342	50.4	159
338	Correlated insulator behaviour at half-filling in magic-angle graphene superlattices. *Nature*, **2018**, 556, 80-84	50.4	1771
337	Unconventional superconductivity in magic-angle graphene superlattices. *Nature*, **2018**, 556, 43-50	50.4	2942
336	Universal behavior of a dispersive Dirac cone in gradient-index plasmonic metamaterials. *Physical Review B*, **2018**, 97,	3.3	3
335	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
334	Implanted neural network potentials: Application to Li-Si alloys. *Physical Review B*, **2018**, 97,	3.3	48
333	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
332	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
331	Dry Dehydrogenation of Ethanol on Pt□u Single Atom Alloys. *Topics in Catalysis*, **2018**, 61, 328-335	2.3	34
330	Electronic structure theory of strained two-dimensional materials with hexagonal symmetry. *Physical Review B*, **2018**, 98,	3.3	37
329	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
328	Compression of Wannier functions into Gaussian-type orbitals. *Computer Physics Communications*, **2018**, 230, 27-37	4.2	2
327	Nonadiabatic Hydrogen Dissociation on Copper Nanoclusters. *Journal of Physical Chemistry Letters*, **2018**, 9, 5339-5343	6.4	7
326	New Pathway for Hot Electron Relaxation in Two-Dimensional Heterostructures. *Nano Letters*, **2018**, 18, 6057-6063	11.5	37
325	Heterointerface effects in the electrointercalation of van der Waals heterostructures. *Nature*, **2018**, 558, 425-429	50.4	125
324	Water facilitates oxygen migration on gold surfaces. *Physical Chemistry Chemical Physics*, **2018**, 20, 2196-2204	3.4	14

323	Density functional theory beyond the Born-Oppenheimer approximation: Accurate treatment of the ionic zero-point motion. *Physical Review B*, **2018**, 98,	3.3	3
322	Relaxation and domain formation in incommensurate two-dimensional heterostructures. *Physical Review B*, **2018**, 98,	3.3	87
321	Dihedral-angle-corrected registry-dependent interlayer potential for multilayer graphene structures. *Physical Review B*, **2018**, 98,	3.3	23
320	Berry curvature dipole current in the transition metal dichalcogenides family. *Physical Review B*, **2018**, 98,	3.3	66
319	Reaction-Induced Excitations and Their Effect on Surface Chemistry. *ACS Catalysis*, **2018**, 8, 10358-10363	13.1	4
318	Lithium Intercalation in Graphene/MoS2 Heterostructures. *Journal of Physical Chemistry C*, **2018**, 122, 24535-24541	3.8	29
317	Anhydrous Methanol and Ethanol Dehydrogenation at Cu(111) Step Edges. *Journal of Physical Chemistry C*, **2018**, 122, 21952-21962	3.8	12
316	Energetics and kinetics of vacancy defects in 4H-SiC. *Physical Review B*, **2018**, 98,	3.3	20
315	Pressure dependence of the magic twist angle in graphene superlattices. *Physical Review B*, **2018**, 98,	3.3	103
314	Quantum plasmons with optical-range frequencies in doped few-layer graphene. *Physical Review B*, **2018**, 97,	3.3	13
313	Emergence and dynamical properties of stochastic branching in the electronic flows of disordered Dirac solids. *Europhysics Letters*, **2018**, 122, 27003	1.6	3
312	Magnetic resonance spectroscopy of an atomically thin material using a single-spin qubit. *Science*, **2017**, 355, 503-507	33.3	74
311	Macroscopic 3D Nanoporosity Formation by Dry Oxidation of AgAu Alloys. *Journal of Physical Chemistry C*, **2017**, 121, 5115-5122	3.8	16
310	Strain effects on the behavior of isolated and paired sulfur vacancy defects in monolayer MoS2. *Physical Review B*, **2017**, 95,	3.3	42
309	Twistronics: Manipulating the electronic properties of two-dimensional layered structures through their twist angle. *Physical Review B*, **2017**, 95,	3.3	171
308	Impact of Vibrations and Electronic Coherence on Electron Transfer in Flat Molecular Wires. *MRS Advances*, **2017**, 2, 811-816	0.7	1
307	Effect of nanoscale flows on the surface structure of nanoporous catalysts. *Journal of Chemical Physics*, **2017**, 146, 214703	3.9	20
306	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

305	Polyiodide-Doped Graphene. *Journal of Physical Chemistry C*, **2017**, 121, 609-615	3.8	19
304	Representations in neural network based empirical potentials. *Journal of Chemical Physics*, **2017**, 147, 024104	3.9	32
303	Nanoribbon edges of transition-metal dichalcogenides: Stability and electronic properties. *Physical Review B*, **2017**, 96,	3.3	15
302	Accurate formation energies of charged defects in solids: A systematic approach. *Physical Review B*, **2017**, 95,	3.3	22
301	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
300	Epsilon-near-zero behavior from plasmonic Dirac point: Theory and realization using two-dimensional materials. *Physical Review B*, **2016**, 94,	3.3	23
299	Controlling O coverage and stability by alloying Au and Ag. *Physical Chemistry Chemical Physics*, **2016**, 18, 26844-26853	3.6	15
298	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
297	Bounds on nanoscale nematicity in single-layer FeSe/SrTiO3. *Physical Review B*, **2016**, 93,	3.3	11
296	Electronic structure theory of weakly interacting bilayers. *Physical Review B*, **2016**, 93,	3.3	114
295	Li intercalation at graphene/hexagonal boron nitride interfaces. *Physical Review B*, **2016**, 93,	3.3	27
294	How Does Nanoporous Gold Dissociate Molecular Oxygen?. *Journal of Physical Chemistry C*, **2016**, 120, 16636-16640	3.8	36
293	Mapping reactive flow patterns in monolithic nanoporous catalysts. *Microfluidics and Nanofluidics*, **2016**, 20, 1	2.8	38
292	MoS Field-Effect Transistor with Sub-10 nm Channel Length. *Nano Letters*, **2016**, 16, 7798-7806	11.5	283
291	Establishing the limits of efficiency of perovskite solar cells from first principles modeling. *Scientific Reports*, **2016**, 6, 36108	4.9	34
290	Noncovalent Bonding Controls Selectivity in Heterogeneous Catalysis: Coupling Reactions on Gold. *Journal of the American Chemical Society*, **2016**, 138, 15243-15250	16.4	35
289	Strain dependence of band gaps and exciton energies in pure and mixed transition-metal dichalcogenides. *Physical Review B*, **2016**, 94,	3.3	72
288	Dumbbell Defects in FeSe Films: A Scanning Tunneling Microscopy and First-Principles Investigation. *Nano Letters*, **2016**, 16, 4224-9	11.5	28

287	Theory of Graphene Raman Scattering. *ACS Nano*, **2016**, 10, 2803-18	16.7	65
286	Catalyst design for enhanced sustainability through fundamental surface chemistry. *Philosophical Transactions Series A, Mathematical, Physical, and Engineering Sciences*, **2016**, 374,	3	13
285	A structural approach to relaxation in glassy liquids. *Nature Physics*, **2016**, 12, 469-471	16.2	214
284	Real-Time TD-DFT with Classical Ion Dynamics: Methodology and Applications. *Journal of Chemical Theory and Computation*, **2016**, 12, 466-76	6.4	41
283	Long-Time Dynamics through Parallel Trajectory Splicing. *Journal of Chemical Theory and Computation*, **2016**, 12, 18-28	6.4	55
282	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
281	Electric field tuning of band offsets in transition metal dichalcogenides. *Physical Review B*, **2016**, 94,	3.3	18
280	Perturbation theory for weakly coupled two-dimensional layers. *Journal of Materials Research*, **2016** , 31, 959-966	2.5	18
279	Direct visualization of quasi-ordered oxygen chain structures on Au(110)-(1 □2). *Surface Science*, **2016**, 650, 5-10	1.8	22
278	Effects of Knudsen diffusivity on the effective reactivity of nanoporous catalyst media. *Journal of Computational Science*, **2016**, 17, 377-383	3.4	34
277	Structural Properties of Defects in Glassy Liquids. *Journal of Physical Chemistry B*, **2016**, 120, 6139-46	3.4	44
276	Enhancing the Hydrogen Activation Reactivity of Nonprecious Metal Substrates via Confined Catalysis Underneath Graphene. *Nano Letters*, **2016**, 16, 6058-6063	11.5	82
275	Superlattice-Induced Insulating States and Valley-Protected Orbits in Twisted Bilayer Graphene. *Physical Review Letters*, **2016**, 117, 116804	7.4	218
274	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
273	High-Temperature Quantum Anomalous Hall Effect in n-p Codoped Topological Insulators. *Physical Review Letters*, **2016**, 117, 056804	7.4	55
272	Atomistic mechanisms for bilayer growth of graphene on metal substrates. *Physical Review B*, **2015**, 91,	3.3	30
271	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
270	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

269	Ab initio tight-binding Hamiltonian for transition metal dichalcogenides. *Physical Review B*, **2015**, 92,	3.3	111
268	Revealing the Empty-State Electronic Structure of Single-Unit-Cell FeSe/SrTiO3. *Physical Review Letters*, **2015**, 115, 017002	7.4	48
267	Identifying structural flow defects in disordered solids using machine-learning methods. *Physical Review Letters*, **2015**, 114, 108001	7.4	206
266	Surface plasmon engineering in graphene functionalized with organic molecules: a multiscale theoretical investigation. *Nano Letters*, **2014**, 14, 50-6	11.5	34
265	Parallel in time approximation of the lattice Boltzmann method for laminar flows. *Journal of Computational Physics*, **2014**, 270, 577-586	4.1	8
264	Structural stability and electronic properties of low-index surfaces of SnS. *Journal of Applied Physics* , **2014**, 115, 173702	2.5	23
263	Graphene/MoS2 hybrid technology for large-scale two-dimensional electronics. *Nano Letters*, **2014**, 14, 3055-63	11.5	472
262	Epitaxial growth of molecular crystals on van der waals substrates for high-performance organic electronics. *Advanced Materials*, **2014**, 26, 2812-7	24	103
261	Qualitative link between work of adhesion and thermal conductance of metal/diamond interfaces. *Journal of Applied Physics*, **2014**, 115, 123509	2.5	34
260	First principles study of point defects in SnS. *Physical Chemistry Chemical Physics*, **2014**, 16, 26176-83	3.6	60
259	Direct observation of a long-lived single-atom catalyst chiseling atomic structures in graphene. *Nano Letters*, **2014**, 14, 450-5	11.5	69
258	Quantum phase transitions and topological proximity effects in graphene nanoribbon heterostructures. *Nanoscale*, **2014**, 6, 3259-67	7.7	8
257	Theory of structural transformation in lithiated amorphous silicon. *Nano Letters*, **2014**, 14, 4065-70	11.5	40
256	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
255	Morphological evolution of Si nanowires upon lithiation: a first-principles multiscale model. *Nano Letters*, **2013**, 13, 2011-5	11.5	39
254	Electrically driven tuning of the dielectric constant in MoS2 layers. *ACS Nano*, **2013**, 7, 10741-6	16.7	146
253	Optoelectronic properties of single-layer, double-layer, and bulk tin sulfide: A theoretical study. *Journal of Applied Physics*, **2013**, 113, 233507	2.5	107
252	Tuning the electronic and chemical properties of monolayer MoS2 adsorbed on transition metal substrates. *Nano Letters*, **2013**, 13, 509-14	11.5	239

251	Electric-field dependence of the effective dielectric constant in graphene. *Nano Letters*, **2013**, 13, 898-902	11.5	147
250	Adsorption and diffusion of lithium on layered silicon for Li-ion storage. *Nano Letters*, **2013**, 13, 2258-63	11.5	299
249	Quasiparticle band structures and interface physics of SnS and GeS. *Physical Review B*, **2013**, 87,	3.3	52
248	Performance Analysis of the Lattice Boltzmann Model Beyond Navier-Stokes **2013**,		29
247	Multiscale Hemodynamics Using GPU Clusters. *Communications in Computational Physics*, **2012**, 11, 48-64	2.4	13
246	Optical and elastic properties of diamond-like carbon with metallic inclusions: A theoretical study. *Journal of Applied Physics*, **2012**, 112, 103503	2.5	28
245	Diffusion of Lithium in Bulk Amorphous Silicon: A Theoretical Study. *Journal of Physical Chemistry C*, **2012**, 116, 22212-22216	3.8	138
244	Ab initio determination of coarse-grained interactions in double-stranded DNA. *Journal of Chemical Physics*, **2012**, 137, 105102	3.9	32
243	Reactive flow in silicon electrodes assisted by the insertion of lithium. *Nano Letters*, **2012**, 12, 4397-403	11.5	145
242	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
241	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
240	Direct imaging of atomic-scale ripples in few-layer graphene. *Nano Letters*, **2012**, 12, 2278-82	11.5	30
239	Theoretical investigation of the C60/copper phthalocyanine organic photovoltaic heterojunction. *Nano Research*, **2012**, 5, 248-257	10	29
238	Topological Graphene Imaging and Fabrication of Devices. *Microscopy and Microanalysis*, **2012**, 18, 1534-1535	0.5	
237	Theoretical Study of O-Assisted Selective Coupling of Methanol on Au(111). *Journal of Physical Chemistry C*, **2011**, 115, 3703-3708	3.8	82
236	Design of Dye Acceptors for Photovoltaics from First-Principles Calculations. *Journal of Physical Chemistry C*, **2011**, 115, 9276-9282	3.8	69
235	Properties of copper (fluoro-)phthalocyanine layers deposited on epitaxial graphene. *Journal of Chemical Physics*, **2011**, 134, 194706	3.9	75
234	D-π-A dye system containing cyano-benzoic acid as anchoring group for dye-sensitized solar cells. *Langmuir*, **2011**, 27, 14248-52	4	39

233	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
232	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
231	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
230	Graphene structures at an extreme degree of buckling. *ACS Nano*, **2011**, 5, 1395-400	16.7	39
229	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
228	Stiffening of organosilicate glasses by organic cross-linking. *Acta Materialia*, **2011**, 59, 44-52	8.4	53
227	Approaching the intrinsic band gap in suspended high-mobility graphene nanoribbons. *Physical Review B*, **2011**, 84,	3.3	32
226	Group theoretical analysis of nitrogen-vacancy center energy levels and selection rules. *Materials Research Society Symposia Proceedings*, **2011**, 1282, 95		
225	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
224	Embrittlement of metal by solute segregation-induced amorphization. *Physical Review Letters*, **2010**, 104, 155502	7.4	58
223	Multiscale Simulation of Cardiovascular flows on the IBM Bluegene/P: Full Heart-Circulation System at Red-Blood Cell Resolution **2010**,		23
222	Graphene hydrate: theoretical prediction of a new insulating form of graphene. *New Journal of Physics*, **2010**, 12, 125012	2.9	38
221	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
220	Electron and hole dynamics in dye-sensitized solar cells: influencing factors and systematic trends. *Nano Letters*, **2010**, 10, 1238-47	11.5	116
219	Electric-field control of magnetism in graphene quantum dots: Ab initio calculations. *Physical Review B*, **2010**, 82, 201411	3.3	38
218	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
217	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
216	Insights from Theory on the Relationship Between Surface Reactivity and Gold Atom Release. *Topics in Catalysis*, **2010**, 53, 365-377	2.3	15

215	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
214	Is the nature of magnetic order in copper-oxides and in iron-pnictides different?. *Solid State Communications*, **2010**, 150, 62-65	1.6	7
213	Hydrokinetic approach to large-scale cardiovascular blood flow. *Computer Physics Communications*, **2010**, 181, 462-472	4.2	52
212	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
211	Theory of spin-conserving excitation of the N-V(-) center in diamond. *Physical Review Letters*, **2009**, 103, 186404	7.4	158
210	MUPHY: A parallel MUlti PHYsics/scale code for high performance bio-fluidic simulations. *Computer Physics Communications*, **2009**, 180, 1495-1502	4.2	101
209	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
208	Nature of Oxidation of the Au(111) Surface: Experimental and Theoretical Investigation. *Journal of Physical Chemistry C*, **2009**, 113, 16561-16564	3.8	41
207	Structural, electronic, and optical properties of representative Cu-flavonoid complexes. *Journal of Physical Chemistry B*, **2009**, 113, 6478-83	3.4	27
206	Atomic Oxygen Adsorption on Au(111) Surfaces with Defects. *Journal of Physical Chemistry C*, **2009**, 113, 3232-3238	3.8	71
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