Group code	Title	Journal	Year	Volume (Issue)	Pages	DOI
blu	Coherent Electron Transport across a 3 nm Bioelectronic Junction Made of Multi-Heme Proteins	J. Phys. Chem. Lett	2020	11	9766-9774	10.1021/acs.jpclett.0c02686
blu	Ergodicity Breaking in Thermal Biological Electron Transfer? Cytochrome C Revisited II	J. Phys. Chem. B}	2020	124	3336-3342	10.1021/acs.jpcb.0c01414
blu	Flickering Polarons Extending over Ten Nanometres Mediate Charge Transport in High-Mobility Organic Crystals	Adv. Theory Simul	2020	3	2000093	10.1002/adts.202000093
blu	Identifying high-mobility tetracene derivatives using a non-adiabatic molecular dynamics approach	J. Mater. Chem. C	2020	8	1054-1064	10.1039/C9TC05270D
blu	Polaronic structure of excess electrons and holes for a series of bulk iron oxides	Phys. Chem. Chem. Phys	2020	22	10699-10709	10.1039/c9cp06482f
blu	Ultrathin porphyrin and tetra-indole covalent organic frameworks for organic electronics applications	J. Chem. Phys.	2020	153	044702	10.1063/5.0010164
blu	Which Multi-Heme Protein Complex Transfers Electrons More Efficiently? Comparing MtrCAB from Shewanella with OmcS from Geobacter	J. Phys. Chem. Lett.	2020	11	9421-9425	10.1021/acs.jpclett.0c02842
cat	A DFT and KMC based study on the mechanism of the water gas shift reaction on the Pd(100) surface	Phys. Chem. Chem. Phys.	2020	22(6)	3620-3632	10.1039/C9CP05476F
cat	Detection of key transient Cu intermediates in SSZ-13 during NH3-SCR deNOx by modulation excitation IR spectroscopy	Chem. Sci.	2020	11	447-455	10.1039/C9SC04905C
cat	Mechanism of CO2 conversion to methanol over Cu (110) and Cu (100) surfaces	Dalton Trans.	2020	49	8478-8497	10.1039/D0DT00754D
cat	Methanol loading dependent methoxylation in zeolite H-ZSM-5	Chem. Sci.	2020	11 (26)	6805-6814	10.1039/D0SC01924K
cat	Modelling the bulk properties of ambient pressure polymorphs of zirconia	Phys. Chem. Chem. Phys.	2020	22(12)	6660-6676	10.1039/D0CP00032A
cat	Morphology of Cu Clusters Supported on Reconstructed Polar ZnO (0001) and (0001 [combining overline]) Surfaces	J. Mater. Chem. A	2020	8 (43	22840-22857	10.1039/D0TA08351H
cat	Synergistic ultraviolet and visible light photo-activation enables intensified low-temperature methanol synthesis over copper/zinc oxide/alumina	Nat. Commun.	2020	11(1)	1-11	10.1038/s41467-020-15445-z
cat/log	Mechanistic Insight into the Framework Methylation of H-ZSM-5 for Varying Methanol Loadings and Si/Al Ratios Using First-Principles Molecular Dy	ACS Catal.	2020	10 (15)	8904-8915	10.1021/acscatal.0c01454
cat/rol	The influence of oxygen vacancy and Ce 3+ ion positions on the properties of small gold clusters supported on CeO 2−x (111)	Journal of Materials Chemistry A	2020	8 (31)	15695-15705	10.1039/D0TA01398F
cat/rol/wil	DFT-Assisted Spectroscopic Studies on the Coordination of Small Ligands to Palladium: From Isolated Ions to Nanoparticles	J. Phys. Chem. C	2020	124(8)	4781-4790	10.1021/acs.jpcc.9b09791
cat/shl	Real and Virtual Polymorphism of Titanium Selenide with Robust Interatomic Potentials	J. Mater. Chem. A	2020	8	14054-14061	10.1039/D0TA03667F
clf	Electron spin mediated distortion in metallic systems	Scripta Materialia	2020	185	159-164	10.1016/j.scriptamat.2020.04.025
cor	Aquaporin-like water transport in nanoporous crystalline layered carbon nitride	Science Advances	2020	6	eabb6011	10.1126/sciadv.abb6011
cor	Diamond-Graphene Composite Nanostructures	Nano Lett	2020	20	3611-3619	10.1021/acs.nanolett.0c00556
~~cor~~	~~Effects of Octahedral Tilting on Band Structure and Thermoelectric Power Factor of Titanate Perovskites: A First-Principles Study on SrTiO3~~	~~J. Phys. Chem. C~~	~~2020~~	~~124~~	~~13045–13052~~	~~10.1021/acs.jpcc.0c03513~~
cor	Enabling stable MnO2 matrix for aqueous zinc-ion battery cathodes	J. Mat. Chem. A	2020	42	22075-22082	10.1039/D0TA08638J
cor	Multi-Scale Investigations of δ-Ni0.25V2O5·nH2O Cathode Materials in Aqueous Zinc-Ion Batteries	Adv Ener Mat	2020	10	2000058	10.1002/aenm.202000058
cre	Adsorption of Aspartic Acid on Ni{100}: A Combined Experimental and Theoretical Study	Langmuir	2020	36 (32)	9399–9411	10.1021/acs.langmuir.0c01175
cre	Molybdenum and sulfur incorporation as oxyanion substitutional impurities in calcium carbonate minerals: A computational investigation	Chem. Geol.	2020	553	119796	10.1016/j.chemgeo.2020.119796
cre	Novel WS2-Based Nanofluids for Concentrating Solar Power: Performance Characterization and Molecular-Level Insights	ACS Appl. Mater. Interfaces	2020	12 (5)	5793–5804	10.1021/acsami.9b18868
cre	The closed-edge structure of graphite and the effect of electrostatic charging	RSC Adv.	2020	10	7994-8001	10.1039/C9RA09913A
cre	Understanding the Specific Heat Enhancement in Metal-Containing Nanofluids for Thermal Energy Storage: Experimental and Ab Initio Evidence for	ACS Appl. Energy Mater.	2020	3 (9)	9246–9256	10.1021/acsaem.0c01556
dos	Optical and Photocatalytic properties of Mixed Anion Solid Solutions: Ba3Sc2-XInXO5Cu2S2 and Ba3In2O5Cu2S2-YSeY	J. Mater. Chem. A	2020	8	19887	10.1039/D0TA06629J
dos	Assessing the Limitations of Transparent Conducting Oxides as Thermoelectrics	J. Mater. Chem. A	2020	8	11948	10.1039/D0TA02247K
dos	Colloidal Synthesis and Optical Properties of Perovskite-Inspired Cesium Zirconium Halide Nanocrystals	ACS Mater. Lett.	2020	2	1644	10.1021/acsmaterialslett.0c00393
dos	Computational Prediction of the Thermoelectric Performance of LaZnOPn (Pn = P, As)	J. Mater. Chem. A.	2020	8	7914	10.1039/D0TA00690D
dos	Computationally Driven Discovery of Layered Quinary Oxychalcogenides: Potential p-Type Transparent Conductors?	Matter	2020	3	759	10.1016/j.matt.2020.05.020
dos	Controlling the thermoelectric properties of organometallic coordination polymers via ligand design	Adv. Funct. Mater.	2020	30	2003106	10.1002/adfm.202003106
dos	Experimental and first-principles spectroscopy of Cu2SrSnS4 and Cu2BaSnS4 photoabsorbers	ACS Appl. Mater. Interfaces	2020	12	50446	10.1021/acsami.0c14578
dos	Geometric analysis and formability of the cubic A2BX6 vacancy ordered double perovskite structure	Chem. Mater.	2020	32	9573	10.1021/acs.chemmater.0c02806
dos	GeSe: optical spectroscopy and theoretical study of a van der Waals solar absorber	Chem. Mater.	2020	32	3245	10.1021/acs.chemmater.0c00453
dos	Identifying Raman Modes of Sb2Se3 and their Symmetries using Angle Resolved Polarised Raman Spectra	J. Mater. Chem. A	2020	8	8337	10.1039/D0TA01783C
dos	Isotype heterojunction solar cells using n-type Sb2Se3 thin films	Chem. Mater.	2020	32	2621	10.1021/acs.chemmater.0c00223
dos	Pronounced Nonlinear Bandgap Behavior in Mixed Cs2Ag(Sb1-xBix)Br6 Double Perovskite Alloys	J. Mater. Chem. A	2020	8	21780	10.1039/D0TA07145E
dos	Resonant doping for high mobility transparent conductors: the case of Mo-doped In2O3	Mater. Horiz.	2020	7	236	10.1039/C9MH01014A
dos	Resonant Ta doping for Enhanced Mobility in Transparent Conducting SnO2	Chem. Mater.	2020	32	1964	10.1021/acs.chemmater.9b04845
dos	Sb 5s2 lone pairs and band alignment of Sb2Se3: a photoemission and density functional theory study	J. Mater. Chem. C	2020	8	12615	10.1039/D0TC03470C
dos	Structure and optical properties of layered perovskite (Ma)2PbI2-xBrx(SCN)2 (0 < x < 1.6)	Inorg. Chem.	2020	59	17379	10.1021/acs.inorgchem.0c02686
dos	Transition Metal Migration Can Facilitate Ionic Diffusion in Defect Garnet Based Intercalation Electrodes	ACS Energy Letters	2020	5	1448	10.1021/acsenergylett.0c00376
dos	Uncovering the origin of the Enhanced Photocatalytic and Antibacterial Ability of Cu-doped TiO2 Thin Films: Theory and Experiment	ACS Appl. Mater. Interfaces	2020	12	15348	10.1021/acsami.9b22056
dos/ske	Polymorph exploration of bismuth stannate using first-principles phonon mode mapping	Chem. Sci.	2020	11	7904-7909	10.1039/D0SC02995E
dos/ske	α-Bi2Sn2O7: a potential room temperature n-type oxide thermoelectric	J. Mater. Chem. A	2020	8	16405-16420	10.1039/D0TA03945D
hep	Calcium-Stannous Oxide Solid Solutions for Solar Devices	Applied Physics Letters	2020	117 (15)	153901-153901	10.1063/5.0024947
hep	ARTEMIS: Ab initio Restructuring Tool Enabling the Modelling of Interface Structures	Computer Physics	2020	257	107515-107515	10.1016/j.cpc.2020.107515
hep	The Potential of Overlayers on Tin-based Perovskites for Water Splitting	The Journal of Physical Chemistry Letters	2020	11 (10)	4124	10.1021/acs.jpclett.0c00964
kos	Evolution of amorphous structure under irradiation: zircon case study	Journal of Physics: Condensed Matter	2020	32	415703	10.1088/1361-648X/ab9f51
kos	Experimental and modeling evidence for structural crossover in supercritical CO2	Phys. Rev. E	2020	101	052109	10.1103/PhysRevE.101.052109
kos	Pronounced structural crossover in water at supercritical pressures	J. Phys. Condens. Matt	2020	32	385102	10.1088/1361-648X/ab94f1
lbp	Pressure−Temperature Phase Diagram of Lithium, Predicted by Embedded Atom Model Potentials	J.Phys.Chem.B.	2020	124	6015−6023	10.1021/acs.jpcb.0c03882
lev	Kinetics of growth of covalent assembly of porphyrin molecules on a copper surface	J. Phys. Chem C	2020	124	22250-22258	10.1021/acs.jpcc.0c02941
lev	Long-range Ordered and Atomic-scale Control of Graphene Hybridization by Photocycloaddition	Nature Chemistry	2020	12	1035 -1041	10.1038/s41557-020-0540-2
lin	Design principles for the ultimate gas deliverable capacity material: nonporous to porous deformations without volume change	Mol. Syst. Des. Eng.	2020	5	1491-1503	10.1039/D0ME00122H
lin	Extracting an Empirical Intermetallic Hydride Design Principle from Limited Data via Interpretable Machine Learning	J. Phys. Chem. Lett.	2020	11	40–47	10.1021/acs.jpclett.9b02971
lin	The Interaction of Hydrogen with the van der Waals Crystal γ-InSe	Molecules	2020	25(11)	2526	10.3390/molecules25112526
log	Methanol loading dependent methoxylation in zeolite H-ZSM-5	Chem. Sci.	2020	11	6805-6814	10.1039/D0SC01924K
log	Polymorphism in a Multicomponent Crystal System of Trimesic Acidand t-Butylamine	Crys. Growth Des.	2020	20	5736-5744	10.1021/acs.cgd.0c00163
lor	Effect of lipid heterogeneity on model human brain lipid membranes	Soft Matter	2020	n/a	n/a	10.1039/D0SM01766C
lor	Morphology of bile salts micelles and mixed micelles with lipolysis products, from scattering techniques and atomistic simulations	J. Colloid. Inter. Sci.	2020	n/a	n/a	10.1016/j.jcis.2020.10.101

lor	Supramolecular architecture of a multi-component biomimetic lipid barrier formulation	J. Coll. Inter. Sci.	2020	n/a	n/a	10.1016/j.jcis.2020.11.017
lor	Understanding the pH-Directed Self-Assembly of a Four-Arm Block Copolymer	Macromolecules	2020	n/a	n/s	10.1021/acs.macromol.0c01694
~~lor~~	~~A pleurocidin analogue with greater conformational flexibility, enhanced antimicrobial potency and in vivo therapeutic efficacy~~	~~Comm. Bio.~~	~~2020~~	~~3~~	~~697~~	~~10.1038/s42003-020-01420-3~~
lor	Accurate large scale modelling of graphene oxide: Ion trapping and chaotropic potential at the interface	Carbon	2020	n/a	n/a	10.1016/j.carbon.2020.12.032
lor	Engineering Chirally Blind Protein Pseudocapsids into Antibacterial Persisters	ACS Nano	2020	14 (2)	1609 – 1622	10.1021/acsnano.9b06814
lor	ILC1 drive intestinal epithelial and matrix remodelling	Nat. Mater	2020	n/a	n/a	10.1038/s41563-020-0783-8
lor	Laurdan and Di-4-ANEPPDHQ Influence the Properties of Lipid Membranes: A Classical Molecular Dynamics and Fluorescence Study	J. Phys. Chem. B	2020	124 (50)	11419–11430	10.1021/acs.jpcb.0c09496
lor	Structure and dynamics of nanoconfined water between surfactant monolayers	Langmuir	2020	36 (1)	447 - 455	10.1021/acs.langmuir.9b03130
lor	Time-resolved fluorescence anisotropy of a molecular rotor resolves microscopic viscosity parameters in complex environments	Small	2020	16 (22)	1907139	10.1002/smll.201907139
lor	Two coexisting membrane structures are defined by lateral and transbilayer interactions between sphingomyelin and cholesterol	Langmuir	2020	36 (33)	9786-9799	10.1021/acs.langmuir.0c01237
~~mat~~	~~CP2K: An electronic structure and molecular dynamics software package - Quickstep: Efficient and accurate electronic structure calculations~~	~~J. Chem. Phys.~~	~~2020~~	~~152~~	~~194103~~	~~10.1063/5.0007045@jcp.2020.ESS2020.issue-1~~
mck	Density Functional Theory and Experimental Determination of Band Gaps and Lattice Parameters in Kesterite Cu2ZnSn(SxSe1–x)4	J. Phys. Chem. Lett.	2020	11	10463	10.1021/acs.jpclett.0c03205
mck	Evidence for self-healing benign grain boundaries and a highly defective Sb2Se3-CdS interfacial layer in Sb2Se3 thin-film photovoltaics	ACS Appl. Mater. Interfaces	2020	12 (19)	21730–21738	10.1021/acsami.0c03690
mck	First-Principles Modelling of Oxygen-Deficient Anatase TiO2 Nanoparticles	J. Phys. Chem. C	2020	124	23637	10.1021/acs.jpcc.0c06052
mol/par	The energetics of carbonated PuO2 surfaces affects nanoparticle morphology: a DFT+U study	Phys. Chem. Chem. Phys.	2020	22	7728-7737	10.1039/D0CP00021C
mur	A point defect model for YBa2Cu3O7 from density functional theory	J. Phys. Commun.	2020	4 (11)	115003	10.1088/2399-6528/abc9a7
mur	Influence of Lithium Vacancy Defects on Tritium Diffusion in β-Li2TiO3	J. Phys. Chem. C	2020	124 (23)	12286–12294	10.1021/acs.jpcc.0c02551
nat	Origin of Solvent-Induced Polymorphism in Self-Assembly of Trimesic Acid Monolayers at Solid–Liquid Interfaces	Chem. Mater.	2020	32 (12)	5057–5065	10.1021/acs.chemmater.0c00827
nik	Adsorption of U(VI) on stoichiometric and oxidised Mackinawite; a DFT Study	Environmental Science and Technology	2020	54	6792–6799	10.1021/acs.est.0c01604
nik	Computational study of plutonium-americium mixed oxides (Pu0.92Am0.08O2-x); water adsorption on (111), (110) and (100) surfaces	J. Phys. Chem. C	2020	124	6646–6658	10.1021/acs.jpcc.9b11601
nik	Formation of a U(VI)-persulfide complex during sulfidation of iron (oxyhydr)oxides	Environmental Science and Technology	2020	54	129–136	10.1021/acs.est.9b03180
pan	Li1.5La1.5MO6 (M = W6+, Te6+) as a new series of lithium-rich double perovskites for all-solid-state lithium-ion batteries,	Nature Communications	2020	11	2041-1723	10.1038/s41467-020-19815-5.
pan	Combined Experimental and Computational Study of Ce-Doped La3Zr2Li7O12 Garnet Solid-State Electrolyte	chemistry of Materials	2020	32	215-223	10.1021/acs.chemmater.9b03526.
pan	Enhancement of photovoltaic efficiency in CdSexTe1−x (where 0≤x≤1): Insights from density functional theory,	J. Phys. Cond. Matter	2020	32	125702 - 125710	10.1088/1361-648x/ab5bba.
pan	Structure and ion transport of lithium-rich Li1+xAlxTi2−x(PO4)3 with 0.3,	Solid State Ionics	2020	346	0167-2738	10.1016/j.ssi.2019.115192
rjm	A deep neural network for molecular wave functions in quasi-atomic minimal basis representation	J. Chem. Phys	2020	153	044123	10.1063/5.0012911
rjm	Alkali doping leads to charge-transfer salt formation in a two-dimensional metal-organic framework	ACS Nano	2020	14 (6)	7475–7483	10.1021/acsnano.0c03133
rjm	Determining the Effect of Hot Electron Dissipation on Molecular Scattering Experiments at Metal Surfaces	JACS Au	2020	1	N/A	10.1021/jacsau.0c00066
rjm	Enhanced Bonding of Pentagon−Heptagon Defects in Graphene to Metal Surfaces: Insights from the Adsorption of Azulene and Naphthalene to Pt(1:	Chem. Matter.	2020	32	1041-1053	10.1021/acs.chemmater.9b03744
rol	Biomass hydrodeoxygenation catalysts innovation from atomistic activity predictors	Philosophical Transactions of the Royal Society A: Ma	2020	378 (2176)	20200056	10.1098/rsta.2020.0056
rol	Mechanistic study of hydrazine decomposition on Ir(111)	Phys. Chem. Chem. Phys.	2020	22	3883-3896	10.1039/C9CP06525C
sal	Calculation of Diamagnetic Susceptibility Tensors of Organic Crystals: From Coronene to Pharmaceutical Polymorphs	J. Phys. Chem. A	2020	124 (7)	1409-1420	10.1021/acs.jpca.9b07104
sal	Reversible, Two-Step Single-Crystal to Single-Crystal Phase Transitions between Desloratadine Forms I, II, and III	Cryst. Growth Des.	2020	20 (3)	1800-1810	10.1021/acs.cgd.9b01522
shl	Modeling of Intrinsic Electron and Hole Trapping in Crystalline and Amorphous ZnO	Advanced Electronic Materials	2020	6 (1)	1900760	10.1002/aelm.201900760
ske	Accuracy of hybrid functionals with non-self-consistent Kohn-Sham orbitals for predicting the properties of semiconductors	J. Chem. Theory. Comput.	2020	16 (6)	3543-3557	10.1021/acs.jctc.9b01218
ske	Assessment of dynamic structural instabilities across 24 cubic inorganic halide perovskites	J. Chem. Phys.	2020	152	10691	10.1063/1.5131575
ske	Lattice dynamics of Pnma Sn(S1-xSex) solid solutions: energetics, phonon spectra and thermal transport	J. Phys.: Energy	2020	2 (2)	10758	10.1088/2515-7655/ab7839
ske	Sn 5s2 lone pairs and the electronic structure of tin sulphides: A photoreflectance, high-energy photoemission, and theoretical investigation	Phys. Rev. Mater.	2020	4 (7)	74602	10.1103/PhysRevMaterials.4.074602
ske/wal	Chemical Trends in the Lattice Thermal Conductivity of Li(Ni, Mn, Co)O2 (NMC) Battery Cathodes	Chem. Mater.	2020	32 (17)	7542–7550	10.1021/acs.chemmater.0c02908

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add	Porosity Switching in Polymorphic Porous Organic Cages with Exceptional Chemical Stability	Angew. Chem. Int. Ed.	2019	58 (13)	4243-4247	10.1002/anie.201813773
add	Redox-Triggered Buoyancy and Size Modulation of a Dynamic Covalent Gel	Chem. Mater.	2019	31 (11)	4148-4155	10.1021/acs.chemmater.9b00919
add	Triazine Functionalized Porous Covalent Organic Framework for Photo-organocatalytic Eâ€“Z Isomerization of Olefins	J. Am. Chem. Soc.	2019	141 (15)	6152-6156	10.1021/jacs.9b01891
blu	Ergodicity-breaking in thermal biological electron transfer? Cytochrome c revisited	J. Phys. Chem. B	2019	123	7588-7598	10.1021/acs.jpcb.9b05253
blu	Kinetics of trifurcated electron flow in the bacterial deca-heme cytochromes MtrC and MtrF	Proc. Nat. Acad. Sci. USA	2019	116	3425-3430	10.1073/pnas.1818003116
blu	Nonadiabatic dynamics with quantum nuclei: Simulating charge transfer with ring polymer surface hopping	Faraday Discuss.	2019	Advance Article	Advance Article	10.1039/C9FD00046A
blu	Quantum localization and delocalization of charge carriers in organic semiconducting crystals	Nature Comm.	2019	10	3843	10.1038/s41467-019-11775-9
blu	Ultra-fast light-driven electron transfer in a Ru(II)tris(bipyridine)-labelled multiheme cytochrome	J. Am. Chem. Soc.	2019	141	15190-15200	10.1021/jacs.9b06858
clf	Interaction of stable aggregates drives the precipitation of calcium phosphate in supersaturated solutions	CrystEngComm	2019	21 (42)	6354-6364	10.1039/c9ce00658c
clo	Self Assembly of Atomically Thin Chiral Copper Heterostructures Templated by Black Phosphorus	Advanced Functional Materials	2019	29 (37)	1903120	10.1002/adfm.201903120
cre	Double-well potential energy surface in the interaction between h-BN and Ni(111)	Phys. Chem. Chem. Phys.	2019	21	10888-10894	10.1039/C8CP07880G
cre	Ensemble-Based Modeling of the NMR Spectra of Solid Solutions:Cation Disorder in Y2(Sn,Ti)2O7	J. Am. Chem. Soc.	2019	141	17838-17846	10.1021/jacs.9b09036
cre	The origin of the vanadium dioxide transition entropy	Phys. Rev. B	2019	99	64113	10.1103/PhysRevB.99.064113
cre	Understanding the origin of disorder in kesterite-type chalcogenides A2ZnBQ4 (A = Cu, Ag; B = Sn, Ge; Q = S, Se): the influence of inter-layer interact	Phys. Chem. Chem. Phys.	2019	21	19311-19317	10.1039/C9CP03630J
dar	Chemical control of structure and guest uptake by a conformationally mobile porous material	Nature	2019	565	213-217	10.1038/s41586-018-0820-9
~~dev~~	~~Anomalous Water and Ion Dynamics in Hydroxyapatite Mesopores~~	~~Computational Materials Science~~	~~2019~~	~~156~~	~~26-34~~	~~10.1016/j.commatsci.2018.08.060~~
dos	An experimental and theoretical study into NaSbS2 as an emerging solar absorber	J. Mater. Chem. C	2019	7	2059	10.1039/C8TC06284F
dos	Anion distribution, structural distortion, and symmetry-driven optical band gap bowing of mixed halide Cs2SnX6 vacancy ordered double perovskite	Chem. Mater.	2019	31	9430	10.1021/acs.chemmater.9b03267
dos	Anionic Order and Band Gap Engineering in Vacancy Ordered Triple Perovskites	Chem. Commun.	2019	55	3164	10.1039/C8CC09947B
dos	Band Edge Evolution of ZnMIII2O4 (MIII = Co, Rh, Ir) Spinels	Phys. Rev. B	2019	100	085126	10.1103/PhysRevB.100.085126
dos	Band Gap, Core-levels and Valence-Band States in Cu3BiS3 for Photovoltaics	ACS Appl. Mater. Interfaces	2019	11	27033	10.1021/acsami.9b04268
dos	Dispelling the Myth of Passivated Codoping in TiO2	Chem. Mater.	2019	31	2577	10.1021/acs.chemmater.9b00257
dos	Electronic band structure and optical properties of boron arsenide	Phys. Rev. Materials	2019	3	51601	10.1103/PhysRevMaterials.3.051601
dos	Exploiting excited-state aromaticity to design highly stable singlet fission materials	J. Am. Chem. Soc.	2019	141	13867	10.1021/jacs.9b06346
dos	Influence of one specific carbonâ€“carbon bond on the quality, stability, and photovoltaic performance of hybrid organicâ€“inorganic bismuthâ€“io	ACS Appl. Energy Mater.	2019	2	1579	10.1021/acsaem.8b01809
dos	Insights into the Electronic Structure of OsO2 using Soft and Hard X-ray Photoelectron Spectroscopy in Combination with Density Functional Theory	Phys. Rev. Mater.	2019	3	25001	10.1103/PhysRevMaterials.3.025001

dos	Intrinsic disorder and the n- and -p-type dopability of the narrow band gap semiconductors GaSb and InSb	Phys. Rev. B	2019	100	035207	10.1103/PhysRevB.100.035207
dos	Origin of High-Efficiency Photoelectrochemical Water Splitting on Hematite/Functional Nanohybrid Metal Oxide Overlayer Photoanode after a Low	ACS Omega	2019	4	1449	10.1021/acsomega.8b02444
dos	Perspectives and Design Principles of Vacancy-Ordered Double Perovskite Halide Semiconductors	Chem. Mater.	2019	31	1184	10.1021/acs.chemmater.8b05036
dos	Sensing and Discrimination of Explosives at Variable Concentrations with a Large-Pore MOF as Part of a Luminescent Array	ACS Appl. Mater. Interfaces	2019	11	11618	10.1021/acsami.8b22385
dos	The complex defect chemistry of Sb2Se3	J. Mater. Chem. A	2019	7	10739	10.1039/C9TA02022E
dos	Two-dimensional eclipsed arrangement hybrid perovskites for tunable energy level alignments and photovoltaics	J. Mater. Chem. C.	2019	7	5139	10.1039/C9TC01325C
ell	Observation of an Inversion in Photophysical Tuning in a Systematic Study of Luminescent Triazole-Based Osmium(II) Complexes	Inorg. Chem.	2019	58 (13)	8607-8621	10.1021/acs.inorgchem.9b00915
gre	Ionic and Electronic Conduction in TiNb2O7	J. Am. Chem. Soc.	2019	141 (42)	16706-16725	10.1021/jacs.9b06669
kos	The nature of collective excitations and their crossover at extreme supercritical conditions	Sci. Rep.	2019	9	755	10.1038/s41598-018-36178-6
kos	Thermodynamic heterogeneity and crossover in the supercritical state of matter	J. Phys. : Condens. Matt.	2019	31	225401	10.1088/1361-648X/ab0ab1
lbp	Thermodynamics and the potential energy landscape: case study of small water clusters	Phys. Chem. Chem. Phys.	2019	21 (14)	7305-7312	10.1039/C9CP00474B
lee	Density functional theory study explaining the underperformance of copper oxides as photovoltaic absorbers	Phys. Rev. B	2019	99 (3)	35154	10.1103/PhysRevB.99.035154
lee	Molecular behaviour of phenol in zeolite Beta catalysts as a function of acid site presence: a quasielastic neutron scattering and molecular dynamics	Catal. Sci. Technol.	2019	9 (23)	6700-6713	10.1039/C9CY01548E
lee	Tuning the electronic band gap of Cu2O via transition metal doping for improved photovoltaic applications	Phys. Rev. B	2019	3 (11)	115202	10.1103/PhysRevMaterials.3.115202
lin	Imaging defects and their evolution in a metal-organic framework at sub-unit-cell resolution	Nature Chemistry	2019	11	622-628	10.1038/s41557-019-0263-4
lin	Kinetic Control of Interpenetration in Fe-Biphenyl-4, 4â€²-Dicarboxylate Metal-Organic Frameworks by Coordination and Oxidation Modulation	J. Am. Chem. Soc.	2019	141	8346-8357	10.1021/jacs.9b03269
lis	Accurate absolute core-electron binding energy of molecules, solids and surfaces from first-principles calculations	Phys. Rev. Materials	2019	3	100801	10.1103/PhysRevMaterials.3.100801
lis	Multiscale modelling of charged impurities in two-dimensional materials	Computational Materials Science	2019	160	368-373	10.1016/j.commatsci.2019.01.012
log	Computational QM/MM investigation of the adsorption of MTH active species in H-Y and H-ZSM-5	Phys. Chem. Chem. Phys.	2019	21	2639	10.1039/C8CP06736H
log	Hybrid-DFT Modeling of Lattice and Surface Vacancies in MnO	J. Phys. Chem. C	2019	123 (13)	8133	10.1021/acs.jpcc.8b07846
log	Main-group test set for materials science and engineering with user-friendly graphical tools for error analysis: systematic benchmark of the numeric	New J. Phys.	2019	21	13025	10.1088/1367-2630/aaf751
log	Polymorphism of lâ€Tryptophan	Angew. Chem. Int. Ed.	2019	131	1	10.1002/anie.201908247
lor	Minor chemistry changes alter surface hydration to control fibronectin adsorption and assembly into nanofibrils	Adv. Theory Sim.	2019	NaN	1900169	10.1002/adts.201900169
lor	Molecular insights into the behaviour of bile salts at interfaces: a key to their role in lipid digestion	J. Colloid Interface Sci	2019	556	266-277	10.1016/j.jcis.2019.08.010
lor	On the hydration of DOPE in solution	J. Chem. Phys.	2019	150	115104	10.1063/1.5085736
lor	On the interaction of hyaluronic acid with synovial fluid lipid membranes	Phys. Chem. Chem. Phys.	2019	21	9845-9857	10.1039/C9CP01532A
lor	On the structure of solid lipid nanoparticles	Small	2019	15	1903156	10.1002/smll.201903156
lor	Targeted fluorescence lifetime probes reveal responsive organelle viscosity and membrane fluidity	PLoS One	2019	14 (2)	e0211165	10.1371/journal.pone.0211165
mck	Electronic Properties of 112 and 110 Twin Boundaries in Anatase TiO2	Adv. Theory Simul.	2019	N/A	1900157	10.1002/adts.201900157
mck	First principles investigation of the structure and properties of Au nanoparticles supported on ZnO	J. Phys. Chem. C	2019	123	21185	10.1021/acs.jpcc.9b02639
mck	First principles investigation of Y2O3-doped HfO2	J. Appl. Phys.	2019	126	84105	10.1063/1.5110669
mck	Forming-Free Grain Boundary Engineered Hafnium Oxide Resistive Random Access Memory Devices	Adv. Electron. Mater.	2019	N/A	1900484	10.1002/aelm.201900484
mck	Passivating Grain Boundaries in Polycrystalline CdTe	J. Phys. Chem. C	2019	123	23882	10.1021/acs.jpcc.9b08373
mck	Screening Doping Strategies to Mitigate Electron Trapping at Anatase TiO2 Surfaces	J. Phys. Chem. C	2019	123	22358	10.1021/acs.jpcc.9b05840
mol	Controlling the {111}/{110} surface Ratio of Cuboidal Ceria Nanoparticles	ACS Appl. Mater. Interfaces	2019	11 (12)	11384-11390	10.1021/acsami.8b21667
mol/par	Computer-Aided Design of Nanoceria Structures as Enzyme Mimetic Agents: The Role of Bodily Electrolytes on Maximising Their Activity	ACS Applied Bio Materials	2019	2 (3)	1098-1106	10.1021/acsabm.8b00709
mol/par	Impact of Hydrogen on the Intermediate Oxygen Clusters and Diffusion in Fluorite Structured UO2+ x	Inorg. Chem.	2019	58 (6)	3774-3779	10.1021/acs.inorgchem.8b03317
muk	Adsorbed States of Hydrogen on Platinum: A New Perspective	Chem Eur J.	2019	25	6496	10.1002/chem.201900351
muk	Identification of normal modes responsible for ferroelectric properties in organic ferroelectric CBDC	J. Phys. Comm.	2019	3	113001	10.1088/2399-6528/ab5431
mur	Visualization of ultrafast melting initiated from radiation-driven defects in solids	Sci. Adv.	2019	5	eaaw0392	10.1126/sciadv.aaw0392
nat	Competitive Metal Coordination of Hexaaminotriphenylene on Cu(111) by Intrinsic Copper Versus Extrinsic Nickel Adatoms	Chem. Eur. J.	2019	25 (8)	1975-1983	10.1002/chem.201803908
nat	Origin of Charge Trapping in TiO2/Reduced Graphene Oxide Photocatalytic Composites: Insights from Theory	ACS Appl. Mater. Interfaces	2019	11 (35)	31909-31922	10.1021/acsami.9b09235
nik	Computational study of the bulk and surface properties of the minor actinide dioxides MAnO2 (MAn = Np, Am, Cm); water adsorption on stoichiome	Journal of Physical Chemistry C	2019	123	15540-15550	10.1021/acs.jpcc.9b02324
pan	Enhanced Li-ion dynamics in trivalently doped Lithium Phosphidosilicate Li2SiP2: A candidate material as a solid li electrolyte,	J. Mater. Chem. A	2019	7	3953-3961	10.1039/c8ta10788b.
par	Defect segregation facilitates oxygen transport at fluorite UO 2 grain boundaries	Philos. Trans. R. Soc. A	2019	377 (2152)	20190026	10.1098/rsta.2019.0026
par	surfinpy: A Surface Phase Diagram Generator	J. Open Source Softw.	2019	4 (34)	1210	10.21105/joss.01210
par/ske	Thermodynamics, Electronic Structure, and Vibrational Properties of Sn n (S 1– x Se x) m Solid Solutions for Energy Applications	Chem. Mater.	2019	31 (10)	3672-3685	10.1021/acs.chemmater.9b00362
pdb	Enhanced visible light absorption for lead-free double perovskite Cs2AgSbBr6	Chem. Commun.	2019	55	3721-3724	10.1039/C9CC01134J
per	Porphine Homocoupling on Au(111)	J. Phys. Chem. C	2019	123	16690-16698	10.1021/acs.jpcc.9b02770
per	Real-Space Observation of Quantum Tunneling by Carbon Atom: Flipping Reaction of Formaldehyde on Cu(110)	The Journal of Physical Chemistry Letter	2019	10	645-649	10.1021/acs.jpclett.8b03806
rjm	Molecular Topology and the Surface Chemical Bond: Alternant Versus Nonalternant Aromatic Systems as Functional Structural Elements	Phys. Rev. X	2019	9	11030	2160-3308/19/9(1)/011030(17)
rjm	Molecule-Metal Bond of Alternant versus Nonalternant Aromatic Systems on Coinage Metal Surfaces: Naphthalene versus Azulene on Ag(111) and (	J. Phys. Chem. C	2019	123	29219-29230	10.1021/acs.jpcc.9b08824
rjm	Unifying machine learning and quantum chemistry with a deep neural network formolecular wavefunctions	Nature Communications	2019	in press	in press	10.1038/s41467-019-12875-2
rol	The Influence of Support Materials on the Structural and Electronic Properties of Gold Nanoparticles â€“ a DFT Study	Phys. Chem. Chem. Phys.	2019	21 (35)	19011-19025	10.1039/C9CP03066B
roy	Can a Single Valence Electron Alter the Electrocatalytic Activity and Selectivity for CO2 Reduction on the Subnanometer Level?	J. Phys. Chem. C	2019	123 (23)	14591-14609	10.1021/acs.jpcc.9b04745
roy	GIGA: A Versatile Genetic Algorithm for Free and Supported Clusters and Nanoparticles in the Presence of Ligands	Nanoscale	2019	11 (18)	9042-9052	10.1039/C9NR02031D
roy	Gold Doping of Tin Clusters: Exo- or Endohedral Complexes	Nanoscale	2019	11 (27)	12878-12888	10.1039/c9nr03233a
roy	Physico-chemical Insights into Gas-phase and Oxide-supported Sub-nanometre AuCu Clusters	, Z. Phys. Chem.	2019	233 (6)	813-843	10.1515/zpch-2018-1356
sal	The (Current) Acridine Solid Form Landscape: Eight Polymorphs and a Hydrate	Crystal Growth & Design	2019	19	4884-4893	10.1021/acs.cgd.9b00557
shl	First principles calculations of optical properties for oxygen vacancies in binary metal oxides	Journ. Chem. Phys.	2019	150 (4)	44702	10.1063/1.5078682
shl	Making amorphous ZnO: Theoretical predictions of its structure and stability	Phys. Rev. B	2019	99 (1)	14202	10.1103/PhysRevB.99.014202
shl	Mechanisms of oxygen vacancy aggregation in SiO2 and HfO2	Frontiers in Physics	2019	7	43	10.3389/fphy.2019.00043
shl	Properties of intrinsic point defects and dimers in hexagonal boron nitride	Jounl Condens. Matter Phys.	2019	32 (5)	55706	10.1088/1361-648X/ab4e5d
shl	Structural, elastic, vibrational and electronic properties of amorphous Sm2O3 from Ab Initio calculations	Comp. Mat. Sci.	2019	169	109119	10.1016/j.commatsci.2019.109119
shl	The origin of negative charging in amorphous Al2O3 films: the role of native defects	Nanotechnology	2019	30 (20)	205201	10.1088/1361-6528/ab0450
ske	Intrinsic Flexibility of the EMT Zeolite Framework under Pressure	Molecules	2019	24 (3)	641	10.3390/molecules24030641
ske	Living in the salt-cocrystal continuum: indecisive organic complexes with thermochromic behaviour	CrystEngComm	2019	21	1626-1634	10.1039/C8CE02066C

ske	Shining Light on Growth-Dependent Surface Chemistry of Organic Crystals: A Polarized Raman Spectroscopic and Computational Study of Aspirin	Cryst. Growth. Des.	2019	19 (2)	1288-1298	10.1021/acs.cgd.8b01693
smw	Are octahedral clusters missing on the carbon energy landscape?	Nanoscale Adv.	2019	1	89-93	10.1039/c8na00013a
sok	Donor and acceptor characteristics of native pointdefects in GaN	J. Phys. D: Appl. Phys.	2019	52 (33)	335104	10.1088/1361-6463/ab2033
sok	Open-Source, Python-Based Redevelopment of the ChemShell Multiscale QM/MM Environment	J. Chem. Theory Comput.	2019	15 (2)	1317-1328	10.1021/acs.jctc.8b01036
str	Nanoparticles actively fragment armored droplets	ACS Nano	2019	13 (8)	9498-9503	10.1021/acsnano.9b04454
wal	Accumulation of Deep Traps at Grain Boundaries in Halide Perovskites	ACS Energy Lett.	2019	4 (6)	1321−1327	10.1021/acsenergylett.9b00840
wal	Anharmonic lattice relaxation during nonradiative carrier capture	Phys. Rev. B	2019	100 (4)	041202(R)	10.1103/PhysRevB.100.041202
wal	Highly Anisotropic Thermal Transport in LiCoO2	J. Phys. Chem. Lett.	2019	10 (18)	5552-5556	10.1021/acs.jpclett.9b02073
wal	Impact of nonparabolic electronic band structure on the optical and transport properties of photovoltaic materials	Phys. Rev. B	2019	99 (8)	85207	10.1103/PhysRevB.99.085207
wal	Lone-pair effect on carrier capture in Cu2ZnSnS4 solar cells	J. Mater. Chem. A	2019	7 (6)	2686-2693	10.1039/c8ta10130b
~~wal~~	~~SMACT: Semiconducting Materials by Analogy and Chemical Theory~~	~~Journal of Open Source Software~~	~~2019~~	~~4 (38)~~	~~1361~~	~~10.21105/joss.01361~~
wal	Stabilization and self-passivation of symmetrical grain boundaries by mirror symmetry breaking	Phys. Rev. Materials	2019	3	14602	10.1103/PhysRevMaterials.3.014602
wil	A combined periodic DFT and QM/MM approach to understand the radical mechanism of the catalytic production of methanol from glycerol.	Farad. Discussions	2019	discussion postpon	N/A	10.1039/D0FD00005A
wil	Photoactive Ag(I)-Based Coordination Polymer as a PotentialSemiconductor for Photocatalytic Water Splitting andEnvironmental Remediation: Expe	J. Phys. Chem. C	2019	123	23940-23950	10.1021/acs.jpcc.9b04957
wil	The Effects of Dopants on the Cu−ZrO2 Catalyzed Hydrogenation ofLevulinic Acid	J. Phys. Chem. C	2019	123	7879-7888	10.1021/acs.jpcc.8b07108
wil	The key role of nanocasting in gold-based Fe2O3 nanocasted catalysts for oxygen activation at the metal-support interface	ChemCatChem	2019	11	1915-1927	10.1002/cctc.201900210

Group code	Title	Journal	Year	Volume (Issue)	Pages	DOI
bjm	Amorphous Sn-Ti Oxides: A Combined Molecular Dynamics and Density Functional Theory Study	Phys. Stat. Sol. A	2018	2018	1800071	10.1002/pssa.201800071
bjm	Controlled Fluorination Reaction of Anatase to Promote Mg2+ Mobility in Rechargeable Magnesium Batteries	Chem. Comm.	2018	54	10080-10083	10.1039/C8CC04136A
bjm	Electronic and Optical Properties of Sodium Niobate: A Density Functional Theory Study	Adv. Mater. Sci. Eng	2018	2018	6416057	10.1155/2018/6416057
bjm	Electronic and optical properties of spinel zinc ferrite: ab initio hybrid functional calculations	J. Phys. Condens. Matter	2018	30	95502	10.1088/1361-648X/aaa7c5
bjm	Interfacial strain effects on lithium diffusion pathways in the spinel solid electrolyte Li-doped MgAl2O4	Phys. Rev. Mater.	2018	2	45403	10.1103/PhysRevMaterials.2.045403
bjm	Lithium Intercalation in Anatase Titanium Vacancies and the Role of Local Anionic Environment	Chem. Mater.	2018	30	3078-3089	10.1021/acs.chemmater.8b00925
bjm	The electrochemical storage mechanism in oxy-hydroxyfluorinated anatase for sodium-ion batteries	Inorg. Chem. Front.	2018	5	1100-1106	10.1039/C8QI00185E
blu	Acidity Constants of the Hematite–Liquid Water Interface from Ab Initio Molecular Dynamics	J. Phys. Chem. Lett	2018	9	5574	10.1021/acs.jpclett.8b01870
blu	Adsorption of amino acids on gold: assessing the accuracy of the GolP-CHARMM forcefield and parametrization of Au-S bonds	J. Chem. Theory Comput.	2018	15	613-624	10.1021/acs.jctc.8b00992
blu	Crossover from hopping to band-like charge transport in an organic semiconductor model: Atomistic non-adiabatic molecular dynamics simulation	J. Phys. Chem. Lett	2018	9	3116-3123	10.1021/acs.jpclett.8b01112
cre	Band Structures of Periodic Porphyrin Nanostructures	J. Phys. Chem. C	2018	122	23790−23798	10.1021/acs.jpcc.8b08131
cre	Combined Experimental and Theoretical Study of Methyl Acetoacetate Adsorption on Ni {100}	J. Phys Chem C	2018	122(11)	6186-6194	10.1021/acs.jpcc.8b00204
cre	Origin of the monolayer Raman signature in hexagonal boron nitride: a first-principles analysis	J. Phys. Condens. Matter	2018	30(18)	185701	10.1088/1361-648X/aab883
dar	Ice nucleation on a corrugated surface	J. Am. Chem. Soc.	2018	140	15804-15811	10.1021/jacs.8b08796
dar	Two-Dimensional Wetting of a Stepped Copper Surface	Phys. Rev. Lett.	2018	120(7)	76101	10.1103/PhysRevLett.120.076101
dev	Solvation and aggregation of meta-aminobenzoic acid in water: density functional theory and molecular dynamics study	Pharmaceutics	2018	10	12	10.3390/pharmaceutics10010012
~~dev~~	~~The role of impurities on the kinetic persistence of amorphous calcium carbonate: a nanoscopic dynamics view~~	~~J. Phys. Chem. C~~	~~2018~~	~~122~~	~~16983-16991~~	~~10.1021/acs.jpcc.8b05189~~
dos	A hard x-ray photoemission study of transparent conducting fluorinedopedtin dioxide	IEEE 7th World Conference on Photovoltaic Energy Cc	2018	3	3051	10.1109/PVSC.2018.8547950
dos	Anharmonicity and Octahedral Tilting in Defect-Ordered Hybrid Perovskites	Chem. Mater.	2018	30	472	10.1021/acs.chemmater.7b04516
dos	Band gap temperature-dependence and exciton-like state in copper antimony sulphide, CuSbS2	APL Mater.	2018	6	84904	10.1063/1.5030207
dos	Cation Size and Cooperative Octahedral Tilting Effects in Vacancy-Ordered Double Perovskite Semiconductors	Chem. Mater.	2018	30	3909	10.1021/acs.chemmater.8b01549
dos	Chemical Vapor Deposition of Photocatalytically Active Pure Brookite Thin films	Chem. Mater.	2018	30	1353	10.1021/acs.chemmater.7b04944
dos	Correlated Polyhedral Rotations in the Absence of Polarons during Electrochemical Insertion of Lithium in ReO3	ACS Energy Lett.	2018	3	2513	10.1021/acsenergylett.8b01179
dos	Deeper Understanding of Interstitial Boron-Doped Anatase Thin Films as A Multifunctional Layer Through Theory and Experiment	J. Phys. Chem. C	2018	122	714	10.1021/acs.jpcc.7b11142
dos	Defect engineering of earth-abundant solar absorbers, BiSI and BiSeI	Chem. Mater.	2018	30	3827	10.1021/acs.chemmater.8b01135
dos	Enhanced electrical properties of antimony doped tin oxide thin films deposited via aerosol assisted chemical vapour deposition	J. Mater. Chem. C	2018	6	7527	10.1039/C8TC01929K
dos	First-Principles Insights into Tin-Based Two-Dimensional Hybrid Halide Perovskites for Photovoltaics	J. Mater. Chem. A	2018	6	5652	10.1039/C8TA00751A
dos	HAXPES-Lab: A laboratory-based Hard X-ray Photoelectron Spectrometer	Rev. Sci. Inst.	2018	89	73105	10.1063/1.5039829
dos	Local corrugation and persistent charge density wave in ZrTe3 with Ni intercalation	Phys. Rev. B	2018	97	155103	10.1103/PhysRevB.97.155103
dos	Phosphorus doped SnO2 thin films for transparent conducting oxide applications: synthesis, optoelectronic properties and computational models	Chem. Sci.	2018	9	7968	10.1039/C8SC02152J
dos	Self-compensation in transparent conductor F-doped SnO2	Adv. Funct. Mater.	2018	28	1701900	10.1002/adfm.201701900
duf	Low temperature ferroelectric behavior in morphotropic Pb (Zr1-xTix)O-3	J. Amer. Ceram. Soc.	2018	101	874-882	10.1111/jace.15101
ell	Mitochondria-localising DNA-binding biscyclometalated phenyltriazole iridium(III) dipyridophenazene complexes: Syntheses and cellular imaging pr	Dalton Trans.	2018	47 (14)	4931-4940	10.1039/C8DT00046H
flo	Thermostatic properties of nitrate molten salts andtheir solar and eutectic mixtures	Scientific Reports	2018	8	10485	10.1038/s41598-018-28641-1
gre	An ab initio investigation on the electronic structure, defect energetics, and magnesium kinetics in Mg3Bi2	J. Mat. Chem. A	2018	6 (35)	16983-16991	10.1039/C7TA11181A
gre	Crystal Structures, Local Atomic Environments, and Ion Diffusion Mechanisms of Scandium-Substituted Sodium Superionic Conductor (NASICON) Sol	Chem. Mater.	2018	30 (8)	2618-2630	10.1021/acs.chemmater.7b05237
gre	Realistic Atomistic Structure of Amorphous Silicon from Machine-Learning-Driven Molecular Dynamics	J. Phys. Chem. Lett.	2018	9 (11)	2879-2885	10.1021/acs.jpclett.8b00902
gre	Structural Characterization of the Li-Ion Battery Cathode Materials LiTixMn(2-x)O4 (0.2 ≤ x ≤ 1.5): A Combined Experimental 7Li NMR and First-Princ	Chem. Mater.	2018	30 (3)	817-829	10.1021/acs.chemmater.7b04314
har	Simulation of Calcium Phosphate Species in Aqueous Solution: Force Field Derivation	J. Phys. Chem. B	2018	122 (4)	1471-1483	10.1021/acs.jpcb.7b10697
jaz	Methyl-rotation dynamics in metal–organic frameworks probed with terahertz spectroscopy	Chem. Commun.	2018	54	5776-5779	10.1039/C8CC02650E
jaz	Predicting the structures and associated phase transition mechanisms in disordered crystals via a combination of experimental and theoretical meth	Faraday Discuss.	2018	211	425-439	10.1039/C8FD00042E
jaz	Revisiting the Thermodynamic Stability of Indomethacin Polymorphs with Low-Frequency Vibrational Spectroscopy and Quantum Mechanical Simul	Cryst. Growth Des.	2018	n/a	in press	10.1021/acs.cgd.8b00623
jaz	Uncovering the Connection Between Low-Frequency Dynamics and Phase Transformation Phenomena in Molecular Solids	Phys. Rev. Lett.	2018	120	196002	10.1103/PhysRevLett.120.196002
kim	A computational exploration of the crystal energy and charge-carrier mobility landscapes of the chiral [6]helicene molecule	Nanoscale	2018	10	1865-1876	10.1039/C7NR08890F
kim	High-throughput discovery of organic cages and catenanes using computational screening fused with robotic synthesis	Nature Commun.	2018	9	2849	10.1038/s41467-018-05271-9
~~kos~~	~~Emergence of microstructure and oxygen diffusion in yttrium-stabilized cubic zirconia~~	~~Phys. Rev. B~~	~~2018~~	~~97~~	~~184107~~	~~10.1103/PhysRevB.97.184107~~
lee	Ab initio investigation of the thermodynamics of cation distribution and of the electronic and magnetic structures in the $LiMn_2O_4$ spinel	Phys. Rev. B	2018	97 (8)	85126	10.1103/PhysRevB.97.085126
lee	CO2 and H2 Adsorption and Reaction at Nin/YSZ(111) Interfaces: A Density Functional Theory Study	The Journal of Physical Chemistry C	2018	122 (34)	19463–19472	10.1021/acs.jpcc.8b03488
lee	Initial Oxygen Incorporation in the Prismatic Surfaces of Troilite FeS	J. Phys. Chem. C	2018	122 (24)	12810-12818	10.1021/acs.jpcc.8b02774

lee	Insight into the Nature of Iron Sulfide Surfaces during the Electrochemical Hydrogen Evolution and CO_2 Reduction Reactions	ACS Appl. Mater. Interfaces	2018	10 (38)	32078–32085	10.1021/acsami.8b08612
lee	Reactivity of CO_2 on the surfaces of magnetite (Fe_3O_4), greigite (Fe_3S_4) and mackinawite (FeS)	Philos. Trans. R. Soc. A Math. Phys. Eng. Sci.	2018	376 (2110)	20170065	10.1098/rsta.2017.0065
lee	Stability and mobility of supported Nin (n = 1–10) clusters on ZrO2(111) and YSZ(111) surfaces: a density functional theory study	Faraday Discussions	2018	208	87-104	10.1039/C7FD00217C
lev	Hydrocarbon decomposition kinetics on the Ir(111) surface	PCCP	2018	20	6083-6099	10.1039/c7cp07526j
lev	Graphene growth by molecular beam epitaxy: an inteplay between desorption, diffusion and intercalation of elemental C species on the islands	Nanoscale	2018	10	7396-7406	10.1039/c8nr00615f
lev	Kinetic control of molecular assembly on surfaces	Communications Chemistry (Nature)	2018	1	166	10.1038/s42004-018-0069-0
lev	On-surface synthesis on a bulk insulator surface	J. Phys.: Cond. Matter	2018	30	133001	10.1088/1361-648X/aab0b9
log	Computational investigation of CO adsorbed on Aux, Agx and (AuAg)x nanoclusters (x=1−5, 147) and monometallic Au and Ag low-energy surfaces	Eur. Phys. J. D	2018	91	32	10.1140/epjb/e2017-80280-7
log	DFT-Computed Trends in the Properties of Bimetallic Precious MetalNanoparticles with Core@Shell Segregation	J. Phys. Chem. C	2018	122	5721-5730	10.1021/acs.jpcc.7b10614
lor	Glycerol solvates DPPC headgroups and localises in the interfacial regions of mod-el pulmonary interfaces altering bilayer structure	Langmuir	2018	34 (23)	6941-6954	10.1021/acs.langmuir.8b00866
lor	Interaction of testosterone-based compounds with dodecyl sulphate monolayers at the air–water interface	Phys. Chem. Chem. Phys.	2018	20	8790 - 8801	10.1039/C7CP07611H
lor	On the hydration structure of the pro-drug GPG-NH2 and its derivatives	Chem. Phys. Lett.	2018	706	228-236	10.1016/j.cplett.2018.05.068
lor	On the solvation of the phosphocholine headgroup in an aqueous propylene glycol solution	J. Chem. Phys.	2018	148	135102	10.1063/1.5024850
lor	PRODAN differentially influences its local environment	Phys. Chem. Chem. Phys.	2018	20	16060-16066	10.1039/C8CP00543E
lor	Proline and water stabilization of a universal two-step folding mechanism for β-turn formation in solution	J. Am. Chem. Soc.	2018	140 (23)	7301-7312	10.1021/jacs.8b03643
lor	Towards optimised drug delivery: structure and composition of testosterone enan-thate in sodium dodecyl sulfate monolayers	Soft Matter	2018	14	3135-3150	10.1039/C7SM01893B
mat/shl	Effect of electric field on migration of defects in oxides: Vacancies and interstitials in bulk MgO	Phys. Rev. B	2018	98	64102	10.1103/PhysRevB.98.064102
mat	Micrometre-long covalent organic fibres by photoinitiated chain-growth radical polymerization on an alkali-halide surface	Nature chemistry	2018	10	1112	10.1038/s41557-018-0120-x
mat/shl	Relation between image charge and potential alignment corrections for charged defects in periodic boundary conditions	J Chem Phys	2018	149	24103	10.1063/1.5029818
mck	Accuracy of electron densities obtained via Koopmans-compliant hybrid functionals	Phys. Rev. Mater. (Rapid comm.).	2018	2	040801(R)	10.1103/PhysRevMaterials.2.040801
mck	Antiphase Boundaries in Truncated Octahedron-shaped Zn-doped Magnetite Nanocrystals	J. Mater. Chem. C	2018	6	12800	10.1039/C8TC05731A
mck	Determination of the structure and properties of an edge dislocation in rutile TiO2	Acta Mater.	2018	163	199	10.1016/j.actamat.2018.10.015
mck	Does Polaronic Self-Trapping Occur at Anatase TiO2 Surfaces?	J. Phys. Chem. C	2018	122	27540	10.1021/acs.jpcc.8b09437
mck	Electronic properties of {111} twin boundaries in a mixed-ion lead halide perovskite solar absorber	ACS Energy Lett.	2018	3	2663	10.1021/acsenergylett.8b01700
mck	Exposure of Mass-Selected Bimetallic Pt-TiO2 to Oxygen explored using the Scanning Transmission Electron Microscopy and Density Functional Theo	RSC Adv.	2018	8	27276	10.1039/C8RA02449A
mck	First principles investigation of titanium nanoparticle oxidation	J. Phys. Chem. C	2018	122	3107	10.1021/acs.jpcc.7b11582
mck	First principles modelling of polaron formation in TiO2 polymorphs	J. Chem. Theory Comput.	2018	14	3740	10.1021/acs.jctc.8b00199
mck	Stability of point defects near MgO grain boundaries in FeCoB/MgO/FeCoB magnetic tunnel junctions	Phys. Rev. Mater.	2018	2	125002	10.1103/PhysRevMaterials.2.125002
mck	Structure and properties of a model conductive filament/host oxide interface in HfO2-based ReRAM	Phys. Rev. Mater.	2018	2	45001	10.1103/PhysRevMaterials.2.045001
mck	Structure, electronic properties and oxygen incorporation/diffusion characteristics of the Σ5 TiN(310) tilt grain boundary	J. Appl. Phys.	2018	123	75301	10.1063/1.5016626
mck	The impact of complex adatom-induced interactions in quantum spin Hall phases	Phys. Rev. B (Rapid comm.)	2018	98	81407	10.1103/PhysRevB.98.081407
mic	Heterogeneous Seeded Molecular Dynamics as a Tool to Probe the Ice Nucleating Ability of Crystalline Surfaces	J. Chem. Phys.	2018	149	72327	10.1063/1.5029336
mon	Charge transfer in trans-combretastatins	Chem. Phys. Lett.	2018	692	146-151	10.1016/j.cplett.2017.12.028
mon	Water Participation in Catalysis: An Atomistic Approach to Solvent Effects in the Catalytic Isomerization of Allylic Alcohols	ACS Catal.	2018	8 (5)	3812-3819	10.1021/acscatal.8b00199
mor	Density functional study of carbon vacancies in titanium carbide	J. Phys. Condens Matter	2018	30	15702	10.1088/1361-648X/aa9979
mos	Mechanisms of reinforcement in polymer nanocomposites	Phys. Chem. Chem. Phys.	2018	20	23085	10.1039/c8cp03281e
mos	Microscopy of hydrogen and hydrogen-vacancy defect structures on graphene devices	Phys. Rev. B	2018	98	155436	10.1103/PhysRevB.98.155436
mos	Tuning electronic properties of transition-metal dichalcogenides via defect charge	Scientific Reports	2018	8	13611	10.1038/s41598-018-31941-1
msa	Pop-On and Pop-Off" Surface Chemistry of Alanine on Ni{111} under Elevated Hydrogen Pressures	The Journal of Physical Chemistry C	2018	122	7720-7730	10.1021/acs.jpcc.8b00186
nik	Multiple water layers on AnO2 {111}, {110} and {100} surfaces (An = U, Pu); A computational study	Journal of Vacuum Science and Technology A	2018	36	41402	10.1116/1.5028210
nik	Oxygen vacancy formation and water adsorption on reduced AnO2 {111}, {110} and {100} surfaces (An = U, Pu); a computational study	Journal of Physical Chemistry C	2018	122	7149–7165	10.1021/acs.jpcc.7b11512
pan	Structure and Lithium-Ion Dynamics in Fluoride-Doped CubicLi7La3Zr2O12 (LLZO) Garnet for Li Solid-State Battery Applications	J. Phys. Chem. C	2018	122	27811-27819	10.1021/acs.jpcc.8b07704
par	The impact of tilt grain boundaries on the thermal transport in perovskite SrTiO 3 layered nanostructures. A computational study	Nanoscale	2018	10 (31)	15010-15022	10.1039/C8NR02234H
par	The critical role of hydrogen on the stability of oxy-hydroxyl defect clusters in uranium oxide	J. Mater. Chem. A	2018	6	11362	10.1039/c8ta02817f
pdb	Fundamental carrier lifetime exceeding 1 µs in Cs2AgBiBr6 double perovskite	Adv. Mater. Interfaces	2018	5	1800464	10.1002/admi.201800464
pdb	Synthesis, crystal structure, magnetic and electronic properties of the caesium-based transition metal halide Cs3Fe2Br9	J. Mat. Chem. C	2018	6	3573-3577	10.1039/c7tc04798c
per	Electric polarisation switching in an atomically-thin binary rock salt structure	Nature Nanotechnology	2018	13, 19-23	19-23	10.1038/s41565-017-0001-2
per	Quantum Tunneling in Real Space: Tautomerization of Single Porphycene Molecules on the (111) Surface of Cu, Ag, and Au	J. Chem. Phys.	2018	148	102330	10.1063/1.5004602
roy	Chemical Bonding in Initial Building Blocks of Semiconductors: Geometrical Structures and Optical Absorption Spectra of Isolated (CdSe2)+ and (Cd2	J. Chem. Phys.	2018	149 (24)	244308	10.1063/1.5066414
roy	Application of a Parallel Genetic Algorithm to the Global Optimization of Medium-sized Au-Pd Sub-nanometre Clusters	Eur. Phys. J. B	2018	19 (2)	34	10.1140/epjb/e2017-80314-2
roy	Effect of Palladium Doping on the Stability and Fragmentation Patterns of Cationic Gold Clusters	Phys. Rev. A	2018	97 (5)	52508	10.1103/PhysRevA.97.052508
roy	First principles global optimization of metal clusters and nanoalloys	Adv. Phys. X	2018	3 (1)	S100009	10.1080/23746149.2018.1516514
roy	Modelling Free and Oxide-supported Nanoalloy Catalysts: Comparison of Bulk-immiscible Pd-Ir and Au-Rh Systems and Influence of a TiO2 Support	Faraday Discussions	2018	208	53-66	10.1039/C7FD00213K
roy	Pentameric PdAu and PdPt nanoparticles on the MgO(1 0 0)surface and their CO and O2 adsorption properties	Eur. Phys. J. B	2018	91 (7)	138	10.1140/epjb/e2018-90060-6
sal	Serendipitous isolation of a disappearing conformational polymorph of succinic acid challenges computational polymorph prediction	CrystEngComm	2018	20 (28)	3971-3977	10.1039/C8CE00625C
sal	Successful Computationally Directed Templating of Metastable Pharmaceutical Polymorphs	Cryst. Growth Des.	2018	18 (9)	5322-5331	10.1021/acs.cgd.8b00765
shl	Identification of oxide defects in semiconductor devices: A systematic approach linking DFT to rate equations and experimental evidence	Microelectronics Reliability	2018	87	286-320	10.1016/j.microrel.2017.12.021
shl	Intrinsic charge trapping in amorphous oxide films: status and challenges	J. Phys.: Condens. Matter	2018	30	233001	10.1088/1361-648X/aac005
shl	Intrinsic electron trapping in amorphous oxides	Nanotech	2018	29	125703	10.1088/1361-6528/aaa77a
shl	Recombination defects at the 4H-SiC/SiO2 interface investigated with electrically detected magnetic resonance and ab initio calculations	Jour. App. Phys.	2018	124	45302	10.1063/1.5024608
shl	Structure and Properties of Intrinsic and Extrinsic Defects in Black Phosphorus	Nanoscale	2018	10	19536-19546	10.1039/c8nr06640j
ske	Acoustic phonon lifetimes limit thermal transport in methylammonium lead iodide	PNAS	2018	115 (47)	11905-11910	10.1073/pnas.1812227115
ske	Hydrogen Bonding versus Entropy: Revealing the Underlying Thermodynamics of the Hybrid Organic–Inorganic Perovskite [CH3NH3]PbBr3	Chemistry of Materials	2018	Article ASAP	Article ASAP	10.1021/acs.chemmater.8b03164
smw	Thermodynamically accessible titanium clusters TiN, N=2-32	Phys. Chem. Chem. Phys.	2018	20 (20)	13962-13973	10.1039/c8cp00406d
sre	Ab initio computer simulations of non-equilibrium radiation-induced cascades in amorphous Ge2Sb2Te5	J. Phys.: Condens. Matter	2018	30 (45)	455401	10.1088/1361-648x/aae340
sre	Modelling the phase-change memory material, Ge2Sb2Te5, with a machine-learned interatomic potential	J. Phys. Chem. B	2018	122 (38)	8998-9006	10.1021/acs.jpcb.8b06476
sre	Origin of radiation tolerance in amorphous Ge2Sb2Te5 phase-change random-access memory material	PNAS	2018	115 (21)	5353-5358	10.1073/pnas.1800638115

Group code	Title	Journal	Year	Volume (Issue)	Pages	DOI
sre	Similarity Between Amorphous and Crystalline Phases: The Case of TiO2	J. Phys. Chem. Lett.	2018	9 (11)	2985–2990	10.1021/acs.jpclett.8b01067
wal	Open-circuit voltage deficit in Cu2ZnSnS4 solar cells by interface bandgap narrowing	Appl. Phys. Lett.	2018	113 (21)	212103	10.1063/1.5063793
wal	Prediction of multiband luminescence due to the gallium vacancy-oxygen defect complex in GaN	Appl. Phys. Lett.	2018	112	262104	10.1063/1.5026751
wal	Stability and electronic properties of planar defects in quaternary I2-II-IV-VI4 semiconductors	J. Appl. Phys.	2018	124 (16)	165705	10.1063/1.5053424
wil	Mechanistic Insights into Selective Oxidation of Polyaromatic Compounds using RICO Chemistry	Chemistry – A European Journal	2018	24	12359-12369	10.1002/chem.201800423
bjm	Self-consistent hybrid functional calculations: Implications for structural, electronic, and optical properties of oxide semiconductors	Nano. Res. Lett.	2017	12	19	10.1186/s11671-016-1779-9
blu	Cysteine linkages accelerate electron flow through tetra-heme protein STC	J. Am. Chem. Soc.	2017	139	17237-17240	10.1021/jacs.7b08831
blu	Detailed balance, internal consistency and energy conservation in fragment orbital-based surface hopping	J. Chem. Phys.	2017	147	214113	10.1063/1.5003820
blu	Electronic couplings for charge transfer across molecule/metal and molecule/semiconductor interfaces: performance of the projector operator-base	J. Phys. Chem. C	2017	121	19677-19689	10.1021/acs.jpcc.7b06566
blu	Improving the performance of hybrid functional-based molecular dynamics simulation through screening of Hartree-Fock exchange forces	J. Chem. Theor. Comput.	2017	13	2178-2184	10.1021/acs.jctc.6b01121
blu	Structure and dynamics at a complex hematite-water interface	J. Am. Chem. Soc.	2017	139	2581-2584	10.1021/jacs.6b13096
cat	A computational study of the heterogeneous synthesis of hydrazine on Co3Mo3N	Catal. Lett.	2017	147	1820-1826	10.1007/s10562-017-2080-y
cat	DFT-D3 study of molecular N2 and H2 activation on Ta3N5 (100), (010) and (001) surfaces	Phys. Chem. Chem. Phys.	2017	19	11968-11974	10.1039/C7CP00806F
clf	A new potential for methyl ammonium lead iodide	Phys. Chem. Chem. Phys.	2017	19	2313	10.1039/c6cp05829a
cor	Phonon-glass electron-crystal Behaviour by A site Disorder in n-Type Thermoelectric Oxides	Energy Environ. Sci.	2017	10	1917-1922	10.1039/C7EE01510K
cre	Crystal structure of cobalt hydroxide carbonate Co2CO3(OH)2: density functional theory and X-ray diffraction investigation	Acta Crystallographica B	2017	73	868–873	10.1107/S2052520617007983
cre	Porphyrin-based metal-organic frameworks for solar fuel synthesis photocatalysis: band gap tuning via iron substitutions	J. Mater. Chem. A	2017	5	11894–11904	10.1039/c7ta01278k
cre	Unsupported trimetallic Ni(Co)-Mo-W sulphide catalysts prepared from mixed oxides: Characterisation and catalytic tests for simultaneous tetralin I	Catalysis Today	2017	292	84-96	10.1016/j.cattod.2016.11.031
dar	Accelerated discovery of two crystal structure types in a complex inorganic phase field	Nature	2017	546	280-284	10.1038/nature22374
dar	Chiral segregation driven by a dynamical response of the adsorption footprint to the local adsorption environment: bitartrate on Cu(110)	Phys. Chem. Chem. Phys.	2017	19	7617--7623	10.1039/c7cp00622e
day	Functional materials discovery using energy-structure-function maps	Nature	2017	543	657-664	10.1038/nature21419
day	Reticular synthesis of porous molecular 1D nanotubes and 3D networks	Nature Chemistry	2017	9	17-25	10.1038/nchem.2663
dos	A Computational and Experimental Study of Ta2O5 Thin Films	J. Phys. Chem. C	2017	121 (1)	202-210	10.1021/acs.jpcc.6b11073
dos	Atypically small temperature-dependence of the direct band gap in the metastable semiconductor copper nitride Cu3N	Phys. Rev. B.	2017	95	115201	10.1103/PhysRevB.95.115201
dos	Chemical Vapor Deposition Synthesis and Optical Properties of Nb2O5 Thin Films with Hybrid Functional Theoretical Insight into the Band Structure	ACS Appl. Mater. Int.	2017	8	18031-18038	10.1021/acsami.7b00907
dos	Core-Levels, Band Alignments, and Valence Band States in CuSbS2 for solar cell applications	ACS Appl. Mater. Interf.	2017	9	4196	10.1021/acsami.7b14208
dos	Electronic and Defect Properties of (CH3NH3)2Pb(SCN)2I2 Analogues for Photovoltaic Applications	J. Mater. Chem. A	2017	5	7845-7853	10.1039/C7TA01688C
dos	Engineering Valence Band Dispersion for High Mobility P-Type Semiconductors	Chem. Mater.	2017	29 (6)	2402-2413	10.1021/acs.chemmater.6b03306
dos	Evidence and effect of photogenerated charge transfer for enhanced photocatalysis in WO3/TiO2 heterojunction films: a computational and experin	Adv. Funct. Mater.	2017	27 (18)	1605413	10.1002/adfm.201605413
dos	Exploring the PbS-Bi2S3 series for next generation energy conversion materials	Chem. Mater.	2017	N/A	N/A	10.1021/acs.chemmater.7b00628
dos	Ising-like antiferromagnetism on the octahedral sublattice of a cobalt-containing garnet and the potential for quantum criticality	Phys. Rev. B	2017	95	144419	10.1103/PhysRevB.95.144419
dos	Narrow-band anisotropic electronic structure of ReS2	Phys. Rev. B	2017	96	85205	10.1103/PhysRevB.96.085205
dos	Transparent conducting n-type ZnO:Sc – synthesis, optoelectronic properties and theoretical insight	J. Mater. Chem. C	2017	5	7585	10.1039/C7TC02389H
dos	Vibronic Structure in the Room Temperature Photoluminescence of the Halide Perovskite Cs3Bi2Br9	Inorg. Chem.	2017	56 (1)	42-45	10.1021/acs.inorgchem.6b01571
duf	Dislocation loop formation by swift heavy ion irradiation of metals	J. Phys.: Condens. Matter	2017	29	285303	10.1088/1361-648X/aa74f8
duf	Improving the Functional Control of Aged Ferroelectrics Using Insights from Atomistic Modeling	Phys. Rev. Lett.	2017	119	117602	10.1103/PhysRevLett.119.177602
duf	Novel high-temperature ferroelectric domain morphology in PbTiO3 ultrathin films	Phys. Chem. Chem. Phys.	2017	19	4243-4250	10.1039/c6cp08157f
ell	Investigation of a new bis(carboxylate)triazole-based anchoring ligand for dye-sensitised solar cell chromophore complexes	Dalton Trans.	2017	X	X	10.1039/c6dt02905a
ell	New cyclometalated iridium(III) dye chromophore complexes for n-type dye-sensitised solar cells	Inorg. Chim. Acta	2017	457	81-89	10.1016/j.ica.2016.12.003
ell	New cyclometalated iridium(III) dye chromophore complexes for p-type dye-sensitised solar cells	Dyes & Pigments	2017	140	269-277	10.1016/j.dyepig.2017.01.011
ell	Theoretical Illumination of Highly Original Photoreactive 3MC States and the Mechanism of the Photochemistry of Ru(II) Tris(bidentate) Complexes	Phys. Chem. Chem. Phys.	2017	19 (40)	27765-27778	10.1039/C7CP05532C
gre	A systematic study of 25Mg NMR in paramagnetic transition metal oxides: applications to Mg-ion battery materials	Phys. Chem. Chem. Phys.	2017	19	613-625	10.1039/C6CP06338A
gre	DFT investigation of the effect of spin-orbit coupling on the NMR shifts in paramagnetic solids	Phys. Rev. B	2017	95	54412	10.1103/PhysRevB.95.054412
gre	Metal–Organic Nanosheets Formed via Defect-Mediated Transformation of a Hafnium Metal–Organic Framework	J. Am. Chem. Soc.	2017	139 (15)	5397-5404	10.1021/jacs.7b00106
gre	Structural simplicity as a restraint on the structure of amorphous silicon	Phys. Rev. B	2017	95	224108	10.1103/PhysRevB.95.224108
gre	Unraveling the Complex Delithiation and Lithiation Mechanisms of the High Capacity Cathode Material V6O13	Chem. Mater.	2017	29 (13)	5513-5524	10.1021/acs.chemmater.7b00428
jam	Atomic structure of Mg-based metallic glasses from molecular dynamics and neutron diffraction	Phys. Chem. Chem. Phys.	2017	19 (12)	8504-15	10.1039/C6CP03261C
jam	Effect of strontium inclusion on the bioactivity of phosphate-based glasses	J. Mat. Sci.	2017	52 (15)	9014-22	10.1007/s10853-017-1155-x
jaz	The significance of the amorphous potential energy landscape for dictating glassy dynamics and driving solid-state crystallisation	Phys. Chem. Chem. Phys.	2017	19	30039-30047	10.1039/C7CP06664C
kim	Computational Screening of Porous Organic Molecules for Xenon/ Krypton Separation	J. Phys. Chem. C	2017	121	15211-15222	10.1021/acs.jpcc.7b03848
kim	Emergent Properties of an Organic Semiconductor Driven by its Molecular Chirality	ACS Nano	2017	11	8329-8338	10.1021/acsnano.7b03540
kim	Reticular synthesis of porous molecular 1D nanotubes and 3D networks	Nature Chemistry	2017	9	17–25	10.1038/nchem.2663
kim	Topological landscapes of porous organic cages	Nanoscale	2017	9	5280-5298	10.1039/c7nr00703e
kos	Direct links between dynamical, thermodynamic, and structural properties of liquids:Modeling results	Phys. Rev. E	2017	95	032116	10.1103/PhysRevE.95.032116
kos	Supercritical Grüneisen parameter and its universality at the Frenkel line	Phys. Rev. E	2017	96	012107	10.1103/PhysRevE.96.012107
kos	Emergence and Evolution of thekGap in Spectra of Liquid and Supercritical States	Phys. Rev. Lett.	2017	118	215502	10.1103/PhysRevLett.118.215502
lee	A Computational Study of the Electronic Properties, Ionic Conduction, and Thermal Expansion of Sm_{1-x}A_xCoO<sub>3</sul	Phys. Chem. Chem. Phys.	2017	19	13960-13969	10.1039/C7CP01555K
lee	Density functional theory study of the zeolite-mediatedtautomerization of phenol and catechol	Mol. Catal.	2017	433	334–345	10.1016/j.mcat.2016.12.020
lee	Density Functional Theory Study of Ni Clusters Supported on the ZrO2(111) Surface	Fuel Cells - From Fundamentals to Systems	2017	17 (2)	125-131	10.1002/fuce.201600044
lee	DFT+U study of the structures and properties of the actinide dioxides	J. Nucl. Mater	2017	492	269-278	10.1016/j.jnucmat.2017.05.025
lee	Modeling of complex interfaces: Gadolinium-doped ceria in contact with yttria-stabilized zirconia	Journal of American Ceramic Society	2017	0	01-Nov	10.1111/jace.14858
lee	Phase stability and thermodynamic properties of FeS polymorphs	J. Phys. Chem. Solids	2017	111	317-323	10.1016/j.jpcs.2017.07.033
lev	A free energy study of carbon clusters on Ir(111): precursors of graphene growth.	J. Chem. Phys.	2017	146	44702	
lev	Ethylene Dissociation on Ni3Al (111)	J. Phys. Chem. C	2017	121	7967–7976	10.1021/acs.jpcc.7b00924
lev	Mechanism of covalent dimerisation on a bulk insulator surface	J. Phys. Chem. C	2017	121	10053-10062	10.1021/acs.jpcc.7b02687

lis	First-principles multiscale modelling of charged adsorbates on doped graphene	2D Materials	2017	4	25070	10.1088/2053-1583/aa6811
lis	Spatially resolving density-dependent screening around a single charged atom in graphene	Phys. Rev. B	2017	95	205419	10.1103/PhysRevB.95.205419
lis	Tuning the Double Layer of Graphene Oxidethrough Phosphorus Doping for EnhancedSupercapacitance	ACS Energy Letters	2017	2	1144-1149	10.1021/acsenergylett.7b00275
log	Magnetic coupling constants for MnO as calculated using hybrid density functional theory	Chem. Phys. Lett.	2017	690	47-53	10.1016/j.cplett.2017.10.027
lor	On the hydration and conformation of cocaine in solution	Chem. Phys. Lett.	2017	676	58-64	10.1016/j.cplett.2017.03.040
lor	Salt interactions in solution prevent urea from direct association with a peptide backbone	J. Phys. Chem. B	2017	121	1866-1876	10.1021/acs.jpcb.6b12542
mck	Atomic structure and electronic properties of MgO grain boundaries in tunnelling magnetoresistive devices	7Scientific Reports	2017	7	45594	10.1038/srep45594
mck	Crystal structure and anti-site boundary defect characterisation in Cu2ZnSnSe4	J. Mater. Chem. A	2017	6	189	10.1039/C7TA08263K
mck	First principles prediction of the morphology of L10 FePt nanoparticles supported on Mg(Ti)O for heat-assisted magnetic recording applications	Phys. Rev. Materials	2017	tbc	tbc	
mic	Communication: Truncated non-bonded potentials can yield unphysicalbehavior in molecular dynamics simulations of interfaces	J. Chem. Phys.	2017	147 (12)	121102	10.1063/1.4997698
mic	Pre-critical fluctuations and what they disclose about heterogeneous crystal nucleation	Nat. Comm.	2017	8	2257	s41467-017-02300-x
mic	Simultaneous Deep Tunneling and Classical Hopping for Hydrogen Diffusion on Metals	Phys. Rev. Lett.	2017	119	126001	10.1103/PhysRevLett.119.126001
mic	What makes a good descriptor for heterogeneous ice nucleation on OH-patterned surfaces	Phys. Rev. B	2017	96 (11)	115441	10.1103/PhysRevB.96.115441
mor	Structure and lattice dynamics of the wide band gap semiconductors MgSiN2 and MgGeN2	J. Appl. Phys.	2017	122	85705	10.1063/1.4985775
mos	First-principles multiscale modelling of charged adsorbates on doped graphene	2D Materials	2017	4	25070	10.1088/2053-1583/aa6811
mos	Molecular Simulation of Gas Solubility in Nitrile Butadiene Rubber	J. Phys. Chem. B	2017	121	287	10.1021/acs.jpcb.6b09690
mos	Spatially resolving density-dependent screening around a single charged atom in graphene	Phys. Rev. B	2017	95	205419	10.1103/PhysRevB.95.205419
msa	The Dynamics of Benzene on Cu(111): a Combined Helium Spin Echo and Dispersion-Corrected DFT Study into the Diffusion of Physisorbed Aromatic	Faraday Discussion	2017	204	471-485	10.1039/C7FD00095B
msa	Ultrafast molecular transport on carbon surfaces: The diffusion of ammonia on graphite	Carbon	2017	126	13-30	10.1016/j.carbon.2017.09.104
nat	Electronic Structure and Charge Transfer in the TiO2 Rutile (110)/Graphene Composite Using Hybrid DFT Calculations	J. Phys. Chem. C	2017	121	4158–4171	10.1021/acs.jpcc.6b12506
nik	Water Adsorption on AnO2 {111}, {110} and {100} Surfaces (An = U and Pu); A Density Functional Theory + U Study	Journal of Physical Chemistry C	2017	121	1675–1682	10.1021/acs.jpcc.6b10986
par	A rapidly-reversible absorptive and emissive vapochromic Pt(II) pincer-based chemical sensor	Nature Comm.	2017	8	1800	10.1038/s41467-017-01941-2
par	Carbonation of Hydrous Materials at the Molecular Level: A Time ofFlight-Secondary Ion Mass Spectrometry, Raman and DensityFunctional Theory S	Cryst. Growth Des.	2017	17	1036-1044	10.1021/acs.cgd.6b01303
par	Exploring Structure-Property Relationships of Silver 4-(Phenylethynyl)pyridine Complexes	Eur. J. Inorg. Chem.	2017	13	1855-1867	10.1002/ejic.201601298
par	Lattice dynamics of the tin sulphides SnS2, SnS and Sn2S3: vibrational spectra and thermal transport	Phys. Chem. Chem. Phys.	2017	19	12452-12465	10.1039/C7CP01680H
par	Structural, Electronic, and Transport Properties of Hybrid SrTiO3-Graphene and Carbon Nanoribbon Interfaces	Chem. Mater.	2017	29 (17)	7364	10.1021/acs.chemmater.7b02253
par	Structure and Properties of Some Layered U2O5 Phases: A DensityFunctional Theory Study	Inorg. Chem.	2017	56	4468-4473	10.1021/acs.inorgchem.7b00014
pdb	Am]Mn(H2POO)3: A New Family of Hybrid Perovskites Based on the Hypophosphite Ligand	JACS	2017	xxx	xxx	10.1021/jacs.7b09417
pdb	Controlling Ag diffusion in ZnO by donor doping: A first principles study	Acta Materialia	2017	137	115-122	10.1016/j.actamat.2017.07.024
per	Desorption of CO from individual ruthenium porphyrin molecules on a copper surface via an inelastic tunnelling process	Chem. Commun.	2017	53	6148-6151	10.1039/c7cc01310h
per	Direct observation of double hydrogen transfer via quantum tunneling in a single porphycene molecule on a Ag(110) surface	Journal of American Chemical Society	2017	139	12681-12687	10.1021/jacs.7b06905
rco	How Inter- and Intramolecular Processes Dictate Aggregation-Induced Emission in Crystals Undergoing Excited-State Proton Transfer	J. Phys. Chem. Lett.	2017	8 (24)	6148-6153	10.1021/acs.jpclett.7b02893
roy	A DFT Study of Molecular Adsorption on Titania-supported AuRh Nanoalloys	Comput. Theor. Chem.	2017	1107	142-151	10.1016/j.comptc.2017.02.012
roy	DFT Global Optimization of Gas-Phase Subnanometer Ru-Pt Clusters	J. Phys. Chem. C	2017	121 (20)	10773-10780	10.1021/acs.jpcc.6b11329
roy	DFT Study of the Structure, Chemical Ordering and Molecular Adsorption of Pd-Ir Nanoalloys	Phys. Chem. Chem. Phys.	2017	19 (39)	27090-27098	10.1039/c7cp04811d
roy	Study of the Stability of Small AuRh Clusters Found by a Genetic Algorithm Methodology	Comp. Theor. Chem.	2017	1119 (1 Nov 2017)	51-58	10.1016/j.comptc.2017.09.008
sal	Thermochemistry of Racemic and Enantiopure Organic Crystals for Predicting Enantiomer Separation	Cryst. Growth Des.	2017	17 (9)	4676–4686	10.1021/acs.cgd.7b00582
shl	A mechanism for Frenkel defect creation in amorphous SiO2 facilitated by electron injection	Nanotech	2017	27	505207	10.1088/0957-4484/27/50/505207
shl	A microscopic mechanism of dielectric breakdown in SiO2 films: An insight from multi-scale modeling	J. App. Phys	2017	121	15501	10.1063/1.4979915
shl	Calculating free energies of organic molecules on insulating substrates	Beilstein J. Nanotech.	2017	8	667-674	10.3762/bjnano.8.71
shl	Defect creation in amorphous HfO2 facilitated by hole and electron injection	Microelectronic Engineering	2017	178	279-283	10.1016/j.mee.2017.05.012
shl	Diffusion and aggregation of oxygen vacancies in amorphous silica	J. Phys.: Condens. Matter	2017	29	245701	10.1088/1361-648X/aa6f9a
shl	Hole trapping in amorphous HfO2 and Al2O3 as a source of positive charging	Microelectronic Engineering	2017	178	235-239	10.1016/j.mee.2017.05.012
shl	Influence of ions on two-dimensional and three-dimensional atomic force microscopy at fluorite-water interfaces	NANOTECHNOLOGY	2017	28	245701	10.1088/1361-6528/aa7188
shl	Interactions of hydrogen with amorphous hafnium oxide	Phys. Rev. B	2017	95	75117	10.1103/PhysRevB.95.075117
shl	Intrinsic resistance switching in amorphous silicon oxide for high performance SiOx ReRAM devices	Microelectron. Eng.	2017	178	98-103	10.1016/j.mee.2017.04.033
shl	Intrinsic Resistance Switching in Amorphous Silicon Suboxides: The Role of Columnar Microstructure	Sci Rep.	2017	7	9274	10.1038/s41598-017-09565-8
shl	Morphology and Growth Mechanisms of Self-Assembled Films on Insulating Substrates: Role of Molecular Flexibility and Entropy	J. Phys. Chem. C	2017	121 (8)	4393–4403	10.1021/acs.jpcc.6b12738
shl	Theoretical modeling of charge trapping in crystalline and amorphous Al2O3	J Phys Condens Matter.	2017	29	314003	10.1088/1361-648X/aa7767
shu	Strain engineering of H/transition metal systems	Surf. Sci.	2017	661	49-59	10.1016/j.susc.2017.03.008
smw	An efficient genetic algorithm for structure prediction at the nanoscale	Nanoscale	2017	9 (11)	3850-3864	10.1039/c6nr09072a
smw	Structure prediction of (BaO)n nanoclusters for n <= 24 evolutionary algorithm	Comp.and Theortical Chem.	2017	1107	74-81	10.1016/j.comptc.2017.01.010
sre	The significance of the amorphous potential energy landscape for dictating glassy dynamics and driving solid-state crystallisation	Phys. Chem. Chem. Phys.	2017	19	30039-30047	10.1039/C7CP06664C
tan	Detecting Molecular Rotational Dynamics Complementing the Low-Frequency Terahertz Vibrations in a Zirconium-Based Metal-Organic Framework	Phys. Rev. Lett.	2017	118	255502	10.1103/PhysRevLett.118.255502
wal	Anharmonic Origin of Giant Thermal Displacements in the Metal–Organic Framework UiO-67	J. Phys. Chem. C	2017	121 (40)	22010–22014	10.1021/acs.jpcc.7b04757
wal	Chemical and Lattice Stability of the Tin Sulfides	J. Phys. Chem. C	2017	12	6446-6454	10.1021/acs.jpcc.6b12581
wal	Chemical bonding at the metal–organic framework/metal oxide interface: simulated epitaxial growth of MOF-5 on rutile TiO2	J. Mater. Chem. A	2017	5 (13)	6226-6232	10.1039/C7TA00356K
wal	Electroactive Nanoporous Metal Oxides and Chalcogenides by Chemical Design	Chem. Mater.	2017	29	3663	10.1021/acs.chemmater.7b00464
wal	H-Centre and V-Centre Defects in Hybrid Halide Perovskites	ACS Energy Lett.	2017	2	2713–2714	10.1021/acsenergylett.7b00995
wal	Quantifying Thermal Disorder in Metal-Organic Frameworks: Lattice Dynamics and Molecular Dynamics Simulations of Hybrid Formate Perovskites	J. Phys. Chem. C	2017	121 (1)	421-429	10.1021/acs.jpcc.6b10714
wal	Spontaneous Octahedral Tilting in the Cubic Inorganic Cesium Halide Perovskites CsSnX3 and CsPbX3 (X = F, Cl, Br, I)	J. Phys. Chem. Lett.	2017	8	4720–4726	10.1021/acs.jpclett.7b02423
wil	The effect of ring size on the selective carboxylation of cycloalkene oxides	Catal. Sci. Technol.	2017	7	1433-1439	10.1039/c6cy02448c
zwi	pH-Directed Aggregation to Control Photoconductivity in Self-Assembled Perylene Bisimides	Chem	2017	2	716-731	10.1016/j.chempr.2017.03.022
zwi	Validating a Density Functional Theory Approach for Predicting the Redox Potentials Associated with Charge Carriers and Excitons in Polymeric Phot	J. Phys. Chem. C	2017	128	1498–1506	10.1021/acs.jpcc.6b11133

Group code	Title	Journal	Year	Volume (Issue)	Pages	DOI
bjm	Influence of Rotational Distortions on Li+ and Na+-Intercalation in Anti-NASICON Fe2(MoO4)3	Chem. Mater	2016	28	4492-4500	10.1021/acs.chemmater.6b01806

bjm	Lithium-ion conductivity in Li6Y(BO3)3: a thermally and electrochemically robust solid electrolyte	J. Mater. Chem. A	2016	4	6972	10.1039/c5ta09436d
bjm	Variation in Surface Energy and Reduction Drive of a Metal Oxide Lithium-Ion Anode with Stoichiometry: a DFT Study of Lithium Titanate Spinel Surf	J. Mater. Chem A	2016	4	17180	10.1039/c6ta05980e
blu	Electronic Coupling Calculations for Bridge-Mediated Charge Transfer Using Constrained Density Functional Theory (CDFT) and Effective Hamiltonia	J. Chem. Theor. Comput.	2016	12	4793-4805	10.1021/acs.jctc.6b00564
blu	Fast interconversion of hydrogen bonding at the hematite(001)-liquid water interface	J. Phys. Chem. Lett.	2016	7	1155	10.1021/acs.jpclett.6b00165
blu	Hematite(001)-liquid water interface from hybrid density functional-based molecular dynamics	J. Phys.: Condens. Matter	2016	28	394001	10.1088/0953-8984/28/39/394001
blu	Mechanism of O2 diffusion and reduction in FeFe hydrogenase	Nat. Chem	2016	Advanced Online	1	10.1038/nchem.2592
cat	Adsorption of formate species on Cu(h,k,l) low index surfaces	Surface Science	2016	653	45-54	10.1016/j.susc.2016.05.002
cat	Band gap reduction in InNxSb1-x alloys: Optical absorption, k.P modeling, and density functional theory	Appl. Phys. Lett.	2016	109	132104	10.1063/1.4963836
cat	Defects and Oxide Ion Migration in the Solid Oxide Fuel Cell Cathode Material LaFeO3	Chem. Mater.	2016	28 (22)	8210-8220	10.1021/acs.chemmater.6b03048
cat	Demonstration of the donor characteristics of Si and O defects in GaN using hybrid QM/MM	Phys. Stat. Solidi A	2016	xx	xx	10.1002/pssa.201600445
cat	DFT-D3 study of molecular N2 and H2 activation on Co3Mo3N surfaces	J. Phys. Chem. C	2016	120	21390–21398	10.1021/acs.jpcc.6b04748
cat	Nonstoichiomety and Weyl fermionic behavior in TaAs	Phys. Rev. B	2016	94	180101(R)	10.1103/PhysRevB.94.18010
cat	Room Tempera ture Methox ylati on in Zeoli tes: In sight into a KeyStep of the Metha nol -to- Hydroc arbons Process	Chem. Comm.	2016	52	2897-2900	10.1039/C5CC08956E
clf	Role of configurational entropy in body-centred cubic or face-centredcubic phase formation in high entropy alloys	Scripta Materialia	2016	124	90-94	10.1016/j.scriptamat.2016.07.001
coo	Ferrous Iron Binding Key to Mms6 Magnetite Biomineralisation: A Mechanistic Study to Understand Magnetite Formation Using pH Titration and NM	Chemistry - A European Journal	2016	22 (23)	7885–7894	0.1002/chem.201600322
cre	Adsorption of Methyl Acetoacetate at Ni{111}: Experiment and Theory	J. Phys. Chem. C	2016	120 (48)	27490–27499	10.1021/acs.jpcc.6b10023
cre	Critical Role of Dynamic Flexibility in Ge-Containing Zeolites: Impact on Diffusion	Chem. Eur. J.	2016	22 (29)	10036–10043	10.1002/chem.201600983
cre	Electron and phonon transport in shandite-structured Ni3Sn2S2	Phys. Rev. B	2016	94 (16)	165131	10.1103/PhysRevB.94.165131
cre	Modelling a Linker Mix-and-Match Approach for Controlling the Optical Excitation Gaps and Band Alignment of Zeolitic Imidazolate Frameworks	Angew. Chem. Int. Ed.	2016	55 (52)	16012-16016	10.1002/anie.201609439
cre	Modelling a Linker Mix-and-Match Approach for Controlling the Optical Excitation Gaps and Band Alignment of Zeolitic Imidazolate Frameworks	Angew. Chem. Int. Ed.	2016	55 (52)	16246–16250	10.1002/anie.201609439
cre	Quantitative Structure of an Acetate Dye Molecule Analogue at the TiO2–Acetic Acid Interface	J. Phys. Chem. C	2016	120 (14)	7586–7590	10.1021/acs.jpcc.6b00186
day	Benchmark fragment-based 1H, 13C, 15N and 17O chemical shift predictions in molecular crystals	Phys. Chem. Chem. Phys.	2016	18	21686-21709	10.1039/C6CP01831A
day	Enhanced NMR Discrimination of Pharmaceutically Relevant Molecular Crystal Forms through Fragment-Based Ab Initio Chemical Shift Predictions	Cryst. Growth Des.	2016	16	6479-6493	10.1021/acs.cgd.6b01157
day	Substituent interference on supramolecular assembly in urea gelators: synthesis, structure prediction and NMR	Soft Matter	2016	12	4034-4043	10.1039/C6SM00607H
dev	Periodic vs. Molecular Cluster Approaches to Resolving Glass Structure and Properties: Anorthite a Case Study	J. Non-Cryst. Solids	2016	451	138–145	10.1016/j.jnoncrysol.2016.06.027
dev	Simulations reveal the role of composition into the predisposed flexibility of bioactive glass ionomer cements	Phys. Chem. Chem. Phys.	2016	8	837-845	10.1039/C5CP05650K
dev	The role of solvent in the self-assembly of m-aminobenzoic acid: a density functional theory and molecular dynamics study	CrystEngComm	2016	18	2937-2948	10.1039/C6CE00130K
dos	An Assessment of Silver Copper Sulphides for Photovoltaic Applications: Theoretical and Experimental Insights	J. Mater. Chem. A	2016	4 (32)	13648-12657	10.1039/C6TA03376H
dos	Assessing the potential of Mg-doped Cr2O3 as a novel p-type transparent conducting oxide	J. Phys.: Condens. Matter	2016	28	125501	10.1088/0953-8984/28/12/125501
dos	Band gap and work function tailoring of SnO2 for improved transparent conducting ability in photovoltaics	J. Mater. Chem. C	2016	4	1467	10.1039/C5TC04089B
dos	Bismuth Oxyhalides: Synthesis, Structure and Photoelectrochemical Activity	Chem. Sci.	2016	7 (8)	4832-4841	10.1039/C6SC00389C
dos	Can Pb-free Halide Double Perovskites Support High-efficiency Solar Cells?	ACS Energy Lett.	2016	1 (5)	949-955	10.1021/acsenergylett.6b00471
dos	Defect Tolerance to Intolerance in the Vacancy Ordered Double Perovskite Semiconductors Cs2SnI6 and Cs2TeI6	J. Amer. Chem. Soc.	2016	138 (27)	8453-8464	10.1021/jacs.6b03207
dos	Direct observation of electrostatically driven band gap renormalization in a degenerate perovskite transparent conducting oxide	Phys. Rev. Lett.	2016	116	27602	10.1103/PhysRevLett.116.027602
dos	Hybrid Organic–Inorganic Coordination Complexes as Tunable Optical Response Materials	Inorg. Chem.	2016	55	3393	10.1021/acs.inorgchem.5b02749
dos	Interplay of Orbital and Relativistic Effects in Bismuth Oxyhalides: BiOF, BiOCl, BiOBr and BiOI	Chem. Mater.	2016	28	1980	10.1021/acs.chemmater.6b00349
dos	Lithium-ion conductivity in Li6Y(BO3)3: a thermally and electrochemically robust solid electrolyte	J. Mater. Chem. A	2016	4	6972	10.1039/C5TA09436D
dos	Modelling potential photovoltaic absorbers Cu3 MCh 4 (M = V, Nb, Ta; Ch = S, Se, Te) using density functional theory	J. Phys.: Condens. Matter	2016	28 (17)	175801	10.1088/0953-8984/28/17/175801
dos	Pilot-Scale Continuous Synthesis of a Vanadium-Doped LiFePO4/C Nanocomposite High-Rate Cathode for Li-Ion Batteries	J. Power Sources	2016	302	410	10.1016/j.jpowsour.2015.10.068
dos	Relativistic electronic structure and band alignment of BiSI and BiSeI: candidate photovoltaic materials	J. Mater. Chem. A	2016	4	2060-2068	10.1039/C5TA09612J
dos	Single Step Solution Processed GaAs Thin Films from GaMe3 and tBuAsH2 Under Ambient Pressure	J. Phys. Chem. C	2016	120	7013	10.1021/acs.jpcc.6b00850
dos	Single-Source Precursor Approach to Aerosol Assisted Chemical Vapour Deposition of Indium Arsenide Thin Films	J. Mater. Chem. C	2016	4 (28)	6761-6768	10.1039/C6TC02293F
dos	Spatial Electron-hole Separation in a One Dimensional Hybrid Organic-Inorganic Lead Iodide	Sci. Rep.	2016	6	20626	10.1038/srep20626
dos	The role of Ni as dopant in Cr2O3: a high figure of merit p-type TCO	J. Mater. Chem. C	2016	5	12610	10.1039/C7TC03545D
dos	The stability of the M2 phase of vanadium dioxide induced by coherent epitaxial strain	Phys. Rev. B	2016	94	85105	10.1103/PhysRevB.94.085105
duf	Contribution of electronic excitation to the structural evolution of ultrafast laser-irradiated tungsten nanofilms	Phys. Rev.B.	2016	93 (10)	104105	10.1103/PhysRevB.93.104105
duf	Modelling the local atomic structure of molybdenum in nuclear waste glasses with ab initio molecular dynamics simulations	Phys. Chem. Chem. Phys.	2016	18 (37)	26125-26132	10.1039/c6cp03076a
duf	Contribution of electronic excitation to the structural evolution of ultrafast laser-irradiated tungsten nanofilms	Phys. Rev. B	2016	93 (10)	104105	10.1103/PhysRevB.93.104105
duf	The influence of the electronic specific heat on swift heavy ion irradiation simulations of silicon.	J.Phys. Cond. Matter	2016	28 (39)	395201	10.1088/0953-8984/28/39/395201
ell	Hybrid cyclometalated iridium coumarin complex as a sensitiser of both n- and p-type DSSCs	Eur. J. Inorg. Chem.	2016	-18	2887–2890	10.1002/ejic.201600242
ell	Luminescent osmium(II) bi-1,2,3-triazol-4-yl complexes: photophysical characterisation and application in light-emitting electrochemical cells	Dalton Trans.	2016	45	7748-7757	10.1039/C6DT00830E
ell	Photochemistry of [Ru(pytz)(btz)2]2+ and characterisation of a κ1-btz ligand-loss intermediate	Inorg. Chem.	2016	55 (15)	7787-7796	10.1021/acs.inorgchem.6b00782
ell	TowardsWater Soluble Mitochondria-Targeting Theranostic Osmium(II) Triazole-Based Complexes	Molecules	2016	21	1382-1394	10.3390/molecules21101382
fou	Ab initio Quantum Monte Carlo Simulation of the Warm Dense Electron Gas in the Thermodynamic Limit	Phys. Rev. Lett.	2016	117	156403	10.1103/PhysRevLett.117.156403
fou	Accurate exchange-correlation energies for the warm dense electron gas	Phys. Rev. Lett.	2016	117	115701	10.1103/PhysRevLett.117.115701
gre	Characterizing Oxygen Local Environments in Paramagnetic Battery Materials via 17O NMR and DFT Calculations	Chem. Mater.	2016	28 (22)	8228-8239	10.1021/acs.chemmater.6b03074
gre	Insights into the Nature and Evolution upon Electrochemical Cycling of Planar Defects in the β-NaMnO2 Na-Ion Battery Cathode: An NMR and First-P	Chem. Mater.	2016	28 (22)	8228-8239	10.1021/acs.chemmater.6b03074
gre	Preventing Structural Rearrangements on Battery Cycling: A First-Principles Investigation of the Effect of Dopants on the Migration Barriers in Layer	J. Phys. Chem. C	2016	120 (35)	19521-19530	10.1021/acs.jpcc.6b05307
gre	Probing Oxide-Ion Mobility in the Mixed Ionic–Electronic Conductor La2NiO4+δ by Solid-State 17O MAS NMR Spectroscopy	J. Am. Chem. Soc.	2016	138 (36)	11958-11969	10.1021/jacs.6b07348
har	Protein Sequences Bound to Mineral Surfaces Persist into Deep Time	eLife	2016	5	e17092	10.7554/eLife.17092
har	Using simulation to understand the structure and properties of hydrated amorphous calcium carbonate	CrystEngComm	2016	18	92-101	10.1039/c5ce01536g
isl	Atomistic Insights into the Oriented Attachment of Tunnel-Based Oxide Nanostructures	ACS Nano	2016	10	539-548	10.1021/acsnano.5b05535
isl	Feeling the strain: enhancing ionic transport in olivine phosphate cathodes for Li- and Na-ion batteries through strain effects	J. Mater. Chem. A	2016	4	6998-7004	10.1039/c5ta09418f
isl	Lattice strain effects on doping, hydration and proton transport in scheelite-type electrolytes for solid oxide fuel cells	Phys. Chem. Chem. Phys	2016	18	29330-29336	10.1039/C6CP06395K
isl	Lithium Extraction Mechanism in Li-Rich Li2MnO3 Involving Oxygen Hole Formation and Dimerization	Chem. Mater.	2016	28	6656–6663	10.1021/acs.chemmater.6b02870
isl	Na2CoSiO4 as a cathode material for sodium-ion batteries: structure, electrochemistry and diffusion pathways	Phys. Chem. Chem. Phys.	2016	18	32744-32752	10.1039/C6CP06777H
isl	The Influence of Large Cations on the Electrochemical Properties of Tunnel-Structured Metal Oxide	Nature Commun	2016	7	13374	10.1038/ncomms13374

jam	Investigating structural features which control the dissolution of bioactive phosphate glasses: Beyond the network connectivity	J. Non-Cryst. Sols.	2016	432A	31-34	10.1016/j.jnoncrysol.2015.01.016
kim	Amine Molecular Cages as Supramolecular Fluorescent Explosive Sensors: A Computational Perspective	J. Phys. Chem. B	2016	120	5063–5072	10.1021/acs.jpcb.6b03059
lee	Photoelectrochemistry: Enhanced Photoresponse of FeS2 Films: The Role of Marcasite–Pyrite Phase Junctions.	Advanced Materials	2016	28 (43)	9656	10.1002/adma.20167030
lee	A combined EXAFS, XRD, DRIFTS and DFT study of nano copper-based catalysts for CO2 hydrogenation	ACS Catalysis	2016	6	5823	10.1021/acscatal.6b01529
lee	A density functional theory study of uranium-doped thoria and uranium adatoms on the major surfaces of thorium dioxide	J. Nucl. Mater.	2016	473	99-111	10.1016/j.jnucmat.2016.02.009
lee	A DFT+U study of the structural, electronic, magnetic, and mechanical properties of cubic and orthorhombic SmCoO3	J. Chem. Phys.	2016	145 (22)	224704	10.1063/1.4971186
lee	Ab initio study of vacancy formation in cubic LaMnO3 and SmCoO3 as cathode materials in solid oxide fuel cells	J. Chem. Phys.	2016	145	14703	10.1063/1.4954939
lee	Calcium Phosphate Prenucleation Complexes in Water by Means of ab Initio Molecular Dynamics Simulations	Cryst. Growth Des.	2016	16 (6)	3353-3358	10.1021/acs.cgd.6b00327
lee	CuO Surfaces and CO2 Activation: A Dispersion-Corrected DFT+ U Study	J. Phys. Chem. C	2016	Just accepted	Just accepted	10.1021/acs.jpcc.5b10431
lee	Density Functional Theory Study of the Adsorption Behaviour of CO2 on Cu2O Surfaces	J. Chem. Phys.	2016	145	44709	10.1063/1.4958804
lee	Density functional theory study of the interaction of H2O, CO2 and CO with the ZrO2 (111), Ni/ZrO2 (111), YSZ (111) and Ni/YSZ (111) surfaces	Surf. Sc.	2016	653	153-162	10.1016/j.susc.2016.06.008
lee	DFT Modeling of the Adsorption of Trimethylphosphine Oxide at theInternal and External Surfaces of Zeolite MFI	J. Phys. Chem. C	2016	120 (34)	19097–19106	10.1021/acs.jpcc.6b03448
lee	DFT-D2 simulations of water adsorption and dissociation on the low-index surfaces of mackinawite (FeS)	J. Chem. Phys.	2016	144	174704	10.1063/1.4947588
lee	DFT-D2 study of the adsorption and dissociation of water on clean and oxygen-covered {001} and {011} surfaces of Mackinawite (FeS).	J. Phys. Chem. C	2016	120 (38)	21441–21450	10.1021/acs.jpcc.6b06122
lee	Early Oxidation Processes on the Greigite Fe_3S_4(001) Surface by Water: A Density Functional Theory Study	J. Phys. Chem. C.	2016	120(16)	8616-8629	10.1021/acs.jpcc.6b00216
lee	Enhanced Photoresponse of FeS2 Films - The Role of Marcasite–Pyrite Phase Junctions.	Advanced Materials	2016	-	-	10.1002/adma.201602222
lee	Mechanistic insights into the Cu(I) Oxide-catalyzed conversion of CO2 to fuels and chemicals: A DFT Approach	Journal of CO2 Utilization	2016	15	96	10.1016/j.jcou.2016.02.008
lee	Surface and shape modification of mackinawite (FeS) nanocrystals by cysteine adsorption - a first-principles DFT-D2 study	Phys. Chem. Chem. Phys.	2016	-	-	10.1039/C6CP05913A
leo	Hierarchical thermoelectrics: crystal grain boundaries as scalable phonon scatterers	Nanoscale	2016	8	3729-3738	10.1039/C5NR05279C
lev	Driving forces for covalent assembly of porphyrins by selective C-H bond activation and intermolecular coupling on a copper surface	JACS	2016	138 (18)	5837–5847	10.1021/jacs.5b11594
lev	Ethylene decomposition on Ir(111): initial path to graphene formation	Phys. Chem. Chem. Phys.	2016	18	27897	10.1039/C6CP03638D
lev	Increasing the templating effect on a bulk insulator surface: from a kinetically trapped to a thermodynamically more stable structure	J. Phys. Chem. C	2016	120	17546	10.1021/acs.jpcc.6b05402
lis	Dispersion and line shape of plasmon satellites in one, two, and three dimensions	Phys. Rev. B	2016	93	235446	10.1103/PhysRevB.93.235446
log	Controlling Structural Transitions in AuAg Nanoparticles through Precise Compositional Design	J. Phys. Chem. Lett	2016	7 (21)	4414	10.1021/acs.jpclett.6b02181
log	Modelling metal centres, acid sites and reaction mechanisms in microporous catalysts	Faraday Discuss.	2016	188	235	10.1039/C6FD00010J
log	Modelling the chemistry of Mn-doped MgO for bulk and (100) surfaces	Phys. Chem. Chem. Phys.	2016	18 (41)	28648	10.1039/C6CP04622C
lor	Atomic scale insights into urea-peptide interactions in solution	Phys. Chem. Chem. Phys.	2016	18	3862-3870	10.1039/C5CP06646H
lor	Comparative atomic-scale hydration of the ceramide and phosphocholine head group in solution and bilayer environments	J. Chem. Phys.	2016	144	225101	10.1063/1.4952444
lor	Specific effects of monovalent counterions on the structural and interfacial properties of dodecyl sulfate monolayers	Phys. Chem. Chem. Phys.	2016	N/A	N/A	10.1039/c6cp05714d
mat	A relationship between three-dimensional surface hydration structures and force distribution measured by atomic force microscopy	Nanoscale	2016	8	7334	10.1039/C5NR08092D
mat	Engineering Polarons at a Metal Oxide Surface	Phys. Rev. Lett.	2016	117	116402	10.1103/PhysRevLett.117.116402
mck	Atomic and electronic structure of twin growth defects in magnetite	Sci. Rep.	2016	6	20943	10.1038/srep20943
mck	Atomic-Scale Structure and Local Chemistry of CoFeB-MgO Magnetic Tunnel Junctions	Nano. Lett.	2016	16	1530	10.1021/acs.nanolett.5b03627
mck	Effect of polaronic charge transfer on band alignment at the Cu/TiO2 interface	Phys. Rev. B	2016	94	155147	10.1103/PhysRevB.94.155147
mck	Modification of charge trapping at particle/particle interfaces by electrochemical hydrogen doping of nanocrystalline TiO2	J. Amer. Chem. Soc.	2016	in press	in press	in press
mck	Origin of Differences in the Excess Volume of Copper and Nickel Grain Boundaries	Acta Mater.	2016	110	246	10.1016/j.actamat.2016.02.040
mck	Polar Spinel-Perovskite Interfaces: an atomistic study of Fe3O4(111)/SrTiO3(111) structure and functionality	Sci. Rep.	2016	6	29724	10.1038/srep29724
mic	Atomic-Scale Picture of the Composition, Decay, and Oxidation of Two-Dimensional Radioactive Films	ACS Nano	2016	10	2152–2158	10.1021/acsnano.5b06640
mic	Can Ice-like Structures Form on Non Ice-like Substrates? The Example of the K-feldspar Microcline	J. Phys. Chem. C	2016	120 (12)	6704–6713	10.1021/acs.jpcc.6b01155
mic	Fast diffusion of water nanodroplets on graphene	Nature Materials	2016	15	66	10.1038/nmat4449
mic	Ice formation on kaolinite: Insights from molecular dynamics simulations	J. Chem. Phys.	2016	145	211927	10.1063/1.4968796
mic	Inverse Temperature Dependence of Nuclear Quantum Effects in DNA Base Pairs	J. Phys. Chem. Lett.	2016	7	2125–2131	10.1021/acs.jpclett.6b00777
mon	Radiation damage in X-ray crystallography: a quantum mechanical study of photoinduced defect formation in beeswax-analogue n-eicosane crystals	Theor. Chem. Acc.	2016	135	01-Oct	10.1007/s00214-015-1779-3
mor	Band gap bowing in NixMg1−xO	Sci. Rep.	2016	6	31230	10.1038/srep31230
mor	Electronic structure of the high and low pressure polymorphs of MgSiN2	Mater. Res. Express	2016	3	85902	10.1088/2053-1591/3/8/085902
mos	Molecular Model for HNBR with Tunable Cross-Link Density	J. Phys. Chem. B	2016	120	12700	10.1021/acs.jpcb.6b07841
msa	Ballistic Diffusion in Polyaromatic Hydrocarbons on Graphite	J. Phys. Chem. Lett.	2016	7	5285-5290	10.1021/acs.jpclett.6b02305
msa	Mass Transport in Surface Diffusion of van der Waals Bonded Systems: Boosted by Rotations?	J. Phys. Chem. Lett.	2016	7	4819-4824	10.1021/acs.jpclett.6b02024
muk	Quasielastic neutron scattering measurements and ab initio MD-simulations on single ion motions in molten NaF	The Journal of Chemical Physics	2016	144	14503	10.1063/1.4939072
nik	Electronic structure of bulk AnO2 (An = U, Np, Pu) and water adsorption on the (111) and (110) surfaces of UO2 and PuO2 from hybrid density functi	J. Nuc. Mat.	2016	482	124–134	10.1016/j.jnucmat.2016.10.005
nik	Ionic adsorption on the brucite (0001) surface: a periodic electrostatic embedded cluster method study	J. Chem. Phys.	2016	145	204708	10.1063/1.4968035
par	An experimental and computational study to resolve the composition of dolomitic lime	RSC Adv.	2016	6	6066-16072	10.1039/C5RA25451E
par	Ba6-3xNd8+2xTi18O54 Tungsten Bronze: A New High-Temperature n-Type Oxide Thermoelectric	J. Electronic. Mater.	2016	45 (3)	1894-1899	10.1007/s11664-015-4275-6
par	Nanostructuring perovskite oxides: the impact of SrTiO3 nanocube 3D self-assembly on thermal conductivity	RSC Adv.	2016	6	114069-114077	10.1039/C6RA23887D
par	Role of Structure and Defect Chemistry in High-Performance Thermoelectric Bismuth Strontium Cobalt Oxides	Chem. Mater.	2016	28 (20)	7470–7478	10.1021/acs.chemmater.6b03200
par	Tungsten Bronze Barium Neodymium Titanate (Ba6–3nNd8+2nTi18O54): An Intrinsic Nanostructured Material and Its Defect Distribution	Inorg. Chem.	2016	55 (7)	3338-3350	10.1021/acs.inorgchem.5b02594
per	Force-induced tautomerization in a single molecule	Nature Chemistry	2016	8	935-940	10.1038/nchem.2552
roy	A Comparative Study of AumRhn (4 <= m+n <= 6) Clusters in the Gas Phase Versus Deposited on (100) MgO	Phys. Chem. Chem. Phys.	2016	18	TBA	10.1039/C6CP03735F
roy	A DFT Study of Molecular Adsorption on Au-Rh Nanoalloys	Cat. Sci. Technol.	2016	6	TBA	10.1039/c6cy01107a
roy	Application of a Parallel Genetic Algorithm to the Global Optimization of Gas-Phase and Supported Gold-Iridium Sub-Nanoalloys	J. Phys. Chem. C	2016	120 (7)	3759-3765	10.1021/acs.jpcc.5b10226
roy	Charge and Compositional Effects on the 2D-3D Transition in Octameric AgAu Clusters	Z. Phys. Chem.	2016	230 (5-7)	955-975	10.1515/zpch-2015-0721
roy	DFT Global Optimisation of Gas-phase and MgO-supported Sub-nanometre AuPd Clusters	Phys. Chem. Chem. Phys.	2016	18 (37)	26133-26143	10.1039/c6cp03958h
roy	Global Optimization of Small Bimetallic Pd-Co Binary Nanoalloy Clusters: A Genetic Algorithm Approach at the DFT Level	Phys. Chem. Chem. Phys.	2016	18 (9)	6676-6682	10.1039/c6cp00342g
roy	Structural Evolution and Metallicity of Lead Clusters	Nanoscale	2016	8 (21)	11153-11160	10.1039/C6NR02080A
roy	Understanding and Controlling the Structure and Segregation Behaviour of AuRh Nanocatalysts	Sci. Rep.	2016	6	35226	10.1038/srep35226
sal	Isomorphous template induced crystallisation: a robust method for the targeted crystallisation of computationally predicted metastable polymorph	Chem. Commun.	2016	52 (46)	7384-7386	10.1039/C6CC01710J
shl	A mechanism for Frenkel defect creation in amorphous SiO2 facilitated by electron injection	Nanotechnology	2016	27	505207	10.1088/0957-4484/27/50/505207

shl	Calculating the Entropy of Adsorption of Organic Molecules at Insulating Surfaces	JPCC	2016	120	3913-3921	10.1021/acs.jpcc.5b12028
shl	Deep electron and hole polarons and bipolarons in amorphous oxide	Phys. Rev. B	2016	94	020103(R)	10.1103/PhysRevB.94.020103
shl	Intrinsic electron traps in atomic-layer deposited HfO2 insulators	Appl. Phys. Lett.	2016	108	222901	10.1063/1.4952718
shl	Nanoscale Transformations in Metastable, Amorphous, Silicon-Rich Silica	Adv. Materials	2016	28	7486-7493	10.1002/adma.201601208
shl	Recombination centers in 4H-SiC investigated by electrically detected magnetic resonance and ab initio modeling	J. Appl. Phys.	2016	119	181507	10.1063/1.4948242
shl	Role of hydrogen in volatile behaviour of defects in SiO2-based electronic devices	Proc. Royal Soc. A	2016	472	20160009	10.1098/rspa.2016.0009
shl	Spectroscopic properties of oxygen vacancies in LaAlO3	Phys. Rev. B	2016	93	134114	10.1103/PhysRevB.93.134114
shl	Structure and luminescence of intrinsic localized states in sodium silicate glasses	Phys. Rev. B	2016	94	174202	10.1103/PhysRevB.94.174202
shu	Non-linear modelling of the effects of strain on transition metal surfaces	Chem. Phys. Letts.	2016	666	51-57	10.1016/j.cplett.2016.10.080
shu	Strain Engineering of the CeNi5 System	Magnetochemistry	2016	2	39	10.3390/magnetochemistry2040039
sok	Double bubble secondary building units used as a structural motif for enhanced electron–hole separation in solids	Materials Science in Semiconductor Processing	2016	42	147-149	10.1016/j.mssp.2015.08.023
wal	A general forcefield for accurate phonon properties of metal-organic frameworks	Phys. Chem. Chem. Phys	2016	18(42)	29316-29329	10.1039/c6cp05106e
wal	Band Alignments, Valence Bands and Core Levels in the Tin Sulfides SnS, SnS2 and Sn2S3: Experiment and Theory	Chem. Mater.	2016	28 (11)	3718-3726	10.1021/acs.chemmater.6b00397
wal	Estimation of semiconductor-like pigment concentrations in paint mixtures and their differentiation from paint layers using first-derivative reflectar	Talanta	2016	154	63-72	10.1016/j.talanta.2016.03.052
wal	Experimental and Theoretical Investigation for Level of Conjugation in Carbazole-based Precursors and their Mono-, Di- and Polynuclear Pt(II) Comp	Inorg. Chem.	2016	Advance Article	Advance Article	10.1021/acs.inorgchem.6b00523
wal	Phonon anharmonicity, lifetimes and thermal transport in CH3NH3PbI3 from many-body perturbation theory	Phys. Rev. B	2016	94 (22)	220301(R)	10.1103/PhysRevB.94.220301
wal	Thermodynamic Origin of Photoinstability in the CH3NH3Pb (I1–x Br x) 3 Hybrid Halide Perovskite Alloy	J. Phys. Chem. Lett.	2016	7 (6)	1083-1087	10.1021/acs.jpclett.6b00226
wat	Modelling potential photovoltaic absorbers Cu3 MCh 4 (M = V, Nb, Ta; Ch = S, Se, Te) using density functional theory	J. Phys. Condens. Matter	2016	28 (17)	175801	10.1088/0953-8984/28/17/175801
wil	CO adsorption over Pd nanoparticles: A general framework for IR simulations on nanoparticles	Surf. Sci.	2016	646	210-220	10.1016/j.susc.2015.07.014
zwi	Controlling Visible Light Driven Photoconductivity in Self-Assembled Perylene Bisimide Structures	J. Phys. Chem. C	2016	120	18479–18486	10.1021/acs.jpcc.6b06222
zwi	Amine Molecular Cages as Supramolecular Fluorescent ExplosiveSensors: A Computational Perspective	J. Phys. Chem. B	2016	120	5063–5072	10.1021/acs.jpcb.6b03059
zwi	Visible-Light-Driven Hydrogen Evolution Using Planarized Conjugated Polymer Photocatalysts	Angew. Chem. Int. Ed.	2016	55 (5)	1792–1796	10.1002/anie.201510542

Group code	Title	Journal	Year	Volume (Issue)	Pages	DOI
ben	Contradistinct Thermoresponsive Behavior of Isostructural MIL-53 Type Metal–Organic Frameworks by Modifying the Framework Inorganic Anion	Chem. Mater.	2015	27 (1)	85-95	10.1021/cm503311x
blu	Electronic couplings for molecular charge transfer: benchmarking CDFT, FODFT and FODFTB against high-level ab initio calculations. II.	Phys. Chem. Chem. Phys	2015	17	14342-14354	10.1039/C4CP04749D
blu	First principles modeling of electron tunneling between defects in m-HfO2	Microelectronic Engineering	2015	147	235–238	10.1016/j.mee.2015.04.009
blu	Flavin binding to the deca-heme cytochrome MtrC: Insights from computational molecular simulation	Biophys. J.	2015	109 (12)	2614-2624	10.1016/j.bpj.2015.10.038
blu	Identification of Mutation Hot-Spots for Substrate Diffusion in Proteins	J. Chem. Theory Comput.	2015	11(4)	1919–1927	10.1021/ct5011455
cat	Buckeridge et al. Reply	Phys. Rev. Lett.	2015	115	29702	10.1103/PhysRevLett.115.029702
cat	Determination of the nitrogen vacancy as a shallow compensating center in GaN doped with divalent metals	Phys. Rev. Lett.	2015	114	16405	10.1103/PhysRevLett.114.016405
cat	Morphological Features and Band Bending at Non-Polar Surfaces of ZnO	Journal of Physical Chemistry C	2015	119 (21)	11598-11611	10.1021/acs.jpcc.5b01331
cat	Nitrogen Activation in a Mars – van Krevelen Mechanism for Ammonia Synthesis on Co3Mo3N	J. Phys. Chem. C	2015	119(51)	28368–28376	10.1021/acs.jpcc.5b06811
cat	Polymorph Engineering of TiO2: Demonstrating How Absolute Reference Potentials Are Determined by Local Coordination	Chem. Mater.	2015	27 (11)	3844-3851	10.1021/acs.chemmater.5b00230
coo	Phage display selected magnetite interactingAdhirons for shape controlled nanoparticlesynthesis	Chemical Science	2015	6	5586-5594	10.1039/C5SC01472G
cor	Importance of anisotropic Coulomb interaction in LaMnO3	Phys. Rev. B	2015	92 (08)	085151-1-16	10.1103/PhysRevB.92.085151
cre	Adsorption of organic molecules at the TiO2(110) surface: the effect of van der Waals interactions	Surf. Sci.	2015	632	142–153	10.1016/j.susc.2014.09.017
cre	Electronic Structure of Pd Multi-Layers on Re(0001): The Role of Charge Transfer	J. Phys. Chem. C	2015	119	23436–23444	10.1021/acs.jpcc.5b06070
cre	Electronic structure of porphyrin-based metal-organic frameworks and their suitability for solar fuel production photocatalysis	J. Mater. Chem. A	2015	3	23458-23465	10.1039/C5TA06982C
cre	Engineering the electronic bandgaps and band edge positions in carbon-substituted 2D boron nitride: a first-principles investigation	Phys. Chem. Chem. Phys.	2015	17 (20)	13547-13552	10.1039/C5CP01680K
cre	The importance of anisotropic Coulomb interaction in LaMnO3	Phys. Rev B	2015	92	85151	10.1103/PhysRevB.92.085151
cre	The interplay of metal-atom ordering, Fermi level tuning and thermoelectric properties in cobalt shandites Co3M2S2 (M = Sn, In)	Chem. Mater.	2015	27	3946–3956	10.1021/acs.chemmater.5b00801
dar	Chemical and Structural Stability of Zirconium-based Metal–Organic Frameworks with Large Three-Dimensional Pores by Linker Engineering	Angew. Chem. Int. Ed.	2015	54	221–226	10.1002/anie.201406501
dar	Computational identification and experimental realization of lithium vacancy introduction into the olivine LiMgPO4	Chem. Mater.	2015	27	2074–2091	10.1021/cm504518q
dar	Tilt engineering of spontaneous polarization and magnetization above 300 K in a bulk layered perovskite	Science	2015	347	420–424	10.1126/science.1262118
dev	Properties of water confined in hydroxy-apatite nanopores as derived from molecular dynamics	Theor. Chem. Acc.	2015	134	59-73	10.1007/s00214-015-1653-3
dos	(CH3NH3)2Pb(SCN)2I2: a more stable structural motif for hybrid halide photovoltaics?	J. Phys. Chem. Lett.	2015	6	4594	10.1021/acs.jpclett.5b02177
dos	Antiferromagnetism at T > 500K in the layered hexagonal ruthenate SrRu2O6	Phys. Rev. B	2015	92	104413	10.1103/PhysRevB.92.104413
dos	Band Gap Dependence on Cation Disorder in ZnSnN2	Adv. Energy Mater.	2015	5	1501462	10.1002/aenm.2015014622
dos	Determination of the nitrogen vacancy as a shallow compensating center in GaN doped with divalent metals	Phys. Rev. Lett.	2015	114	16405	10.1103/PhysRevLett.114.016405
dos	Electronic and surface properties of Ga-doped In2O3 ceramics	Appl. Surf. Sci.	2015	349	970–982	10.1016/j.apsusc.2015.04.106
dos	Interfacial effects in e-LixVOPO4 and evolution of the electronic structure	Chem. Mater.	2015	27	8211	10.1021/acs.chemmater.5b021458
dos	Multifunctional P-doped TiO2 Films: A New Approach to Self-Cleaning, Transparent Conducting Oxide Materials.	Chem. Mater.	2015	27	3234–3242	10.1021/cm504734a
dos	Origin of High Mobility in Molybdenum-Doped Indium Oxide	Chem. Mater.	2015	27 (8)	2788–2796	10.1021/cm503896h
dos	Polymorph Engineering of CuMO2 (M=Al, Ga, Sc, Y) Semiconductors for Solar Energy Applications: From Delafossite to Wurtzite	Acta Cryst. Sec. B	2015	B71	702	10.1107/S2052520615018387
dos	Scalable Route to CH3NH3PbI3 Perovskite Thin Films by Aerosol Assisted Chemical Vapor Deposition	J. Mater. Chem. A.	2015	3 (17)	9071-9073	10.1039/C4TA05522E
dos	Self-regulation mechanism for charged point defects in hybrid halide perovskites	Angew. Chem. Intl. Ed.	2015	54	1791-1794	10.1002/anie.201409740
dos	The electronic structure of sulvanite structured semiconductors Cu3MCh4 (M = V, Nb, Ta; Ch = S, Se, Te): Prospects for optoelectronic applications,	J. Mater. Chem. C	2015	6	12236	10.1039/C5TC02760H
dos	The Origin of High Mobility in Molybdenum Doped Indium Oxide	Chem. Mater.	2015	27	2788–2796	10.1021/cm503896h
dos	The vapour phase detection of explosive markers and derivatives using two fluorescent metal-organic frameworks	J. Mater. Chem. A.	2015	3 (12)	6351-6359	10.1039/C4TA05638H
duf	Dynamical simulations of an electronically induced solid-solid phase transformation in tungsten	Phys. Rev. B	2015	92	134110	10.1103/Phys.RevB.92.134110
duf	Mechanims of helium accomodation in lithium metatitanate	Fus. Eng. Des.	2015	101	94-100	10.1016/j.fusenddes.2015.10.007
duf	Shell model force-field for lead zirconate titanatePb(Zr1.xTix)O3	J. Phys. Chem. C	2015	119 (31)	17784–17789	10.1021/acs.jpcc.5b03207
duf	Structure and ionic diffusion of alkaline-earth ions in mixed cation glasses A(2)O-2MO-4SiO(2) with molecular dynamics simulations	J. Non-Cryst. Solids	2015	422	57-63	10.1016/j.jnoncrysol.2015.05.005
fou	Interaction picture density matrix quantum Monte Carlo	J. Chem. Phys.	2015	143	44116	10.1063/1.4927434
fou	Open-source development experiences in scientific software: the HANDE quantum Monte Carlo project.	J. Open Res. Software	2015	3	e9	10.5334/jors.bw
fou	Systematic study of finite-size effects in quantum Monte Carlo calculations of real metallic systems	J. Chem. Phys.	2015	143	102807	10.1063/1.4922619

gre	Mapping Structural Changes in Electrode Materials: Application of the Hybrid Eigenvector-Following Density Functional Theory (DFT) Method to Lay	Chem. Mater.	2015	12 (16)	5550-5561	10.1021/acs.chemmater.5b01674
gre	Review—Manganese-Based P2-Type Transition Metal Oxides as Sodium-Ion Battery Cathode Materials	J. Electrochem. Soc.	2015	162 (14)	A2589–A2604	10.1149/2.0201514jes
har	Adsorption of poly acrylic acid onto the surface of calcite: an experimental and simulation study	PHYSICAL CHEMISTRY CHEMICAL PHYSICS	2015	17 (41)	27357-27365	10.1039/c5cp00945f
har	How does an amorphous surface influence molecular binding? - ovocleidin-17 and amorphous calcium carbonate	PHYSICAL CHEMISTRY CHEMICAL PHYSICS	2015	17 (26)	17494-17500	10.1039/c5cp00434a
isl	Ionic transport in hybrid lead iodide perovskite solar cells	Nature Communications	2015	6	7497	10.1038/ncomms8497
isl	Sodium-Ion Diffusion and Voltage Trends in Phosphates Na4M3(PO4)2P2O7 (M = Fe, Mn, Co, Ni) for Possible High Rate Cathodes	J. Phys. Chem. C	2015	119	15935-15941	10.1021/acs.jpcc.5b04648
isl	Structural and Mechanistic Insights into Fast Lithium-Ion Conduction in Li4SiO4-Li3PO4 Solid Electrolytes	J. Am. Chem. Soc.	2015	137	9136-9145	10.1021/jacs.5b04444
isl	Unusual Mn Coordination and Redox Chemistry in the High Capacity Borate Cathode Li7Mn(BO3)3	Phys. Chem. Chem. Phys.	2015	17	22259-22265	10.1039/C5CP02711J
kim	Predicting solvent effects on the structure of porous organic molecules	Chem. Commun.	2015	51	15542	10.1039/c5cc05344g
kim	Tunable Porosity through Cooperative Diffusion in a Multicomponent Porous Molecular Crystal	J. Phys. Chem. C	2015	119	22577-22586	10.1021/acs.jpcc.5b07200
kos	Electronic effects in high-energy radiation damage in tungsten	Journal of Physics: Condensed Matter	2015	27	135401	10.1088/0953-8984/27/13/135401
kos	Frenkel line and solubility maximum in supercritical fluids	Phys. Rev. E	2015	91	012112	10.1103/PhysRevE.91.012112
lee	Activation and dissociation of CO2 on the (001), (011), and (111) surfaces of mackinawite (FeS): A dispersion-corrected DFT study	J. Phys. Chem.	2015	143	094703-8	10.1063/1.4929470
lee	Bio-inspired CO2 conversion by iron sulfide catalysts under sustainable conditions	Chem Commun	2015	51 (35)	7501-4	10.1039/c5cc02078f
lee	Configurational analysis of uranium-doped thorium dioxide	2015 IOP Conf. Ser.: Mater. Sci. Eng.	2015	80 (1)	12007	10.1088/1757-899X/80/1/012007
lee	Density functional theory calculations of the hydrazine decomposition mechanism on the planar and stepped Cu(111) surfaces	Phys Chem Chem Phys	2015	17 (33)	21533-46	10.1039/c5cp03204k
lee	Density functional theory study of the effect of helium clusters on tritium-containing palladium lattices	J. Phys.: Condens. Matter	2015	27 (47)	475002	10.1088/0953-8984/27/47/475002
lee	Effect of Chondroitin 4-Sulfate on the Growth and Morphology ofCalcium Oxalate Monohydrate: A Molecular Dynamics Study	Cryst. Growth Des	2015	15 (9)	4438–4447	10.1021/acs.cgd.5b00747
lee	First-principles study of the inversion thermodynamics and electronic structure of FeM2X4 (thio)spinels (M = Cr,Mn, Co, Ni; X = O, S)	Phys. Rev. B.	2015	91(19)	195106	10.1103/PhysRevB.91.195106
lee	Gadolinium-Vacancy Clusters in the (111) Surface of Gadolinium-Doped Ceria: A Density Functional Theory Study	Chem. Mater.	2015	27	7910-7917	10.1021/acs.chemmater.5b02861
lee	Hydrazine network on Cu(111) surface: A Density Functional Theory approach	Surf. Sci.	2015	637-638	140–148	10.1016/j.susc.2015.04.001
lee	Investigating structural features which control the dissolution of bioactive phosphate glasses: Beyond the network connectivity	J. Non-Cryst. Sols.	2015	432 (Part A)	31-34	10.1016/j.jnoncrysol.2015.01.016
lee	Multichannel Detection and Differentiation of Explosives with a Quantum Dot Array	ACS Nano	2015	10 (1)	1139-46	10.1021/acsnano.5b06433
lee	Ni Deposition on Yttria-Stabilized ZrO2(111) Surfaces: A Density Functional Theory Study	J. Phys. Chem. C	2015	119 (12)	6581-6591	10.1021/jp512594j
lee	Preferential sites for intra-molecularglucosepane cross-link formation in type I collagen: A thermodynamic study.	Matrix Biol.	2015	48	78-88	10.1016/j.matbio.2015.06.001
lee	The effect of water on the binding of glycosaminoglycan saccharides to hydroxyapatite surfaces: a molecular dynamics study	Phys. Chem. Chem. Phys.	2015	17	22377-22388	10.1039/C5CP02630J
lee	Theoretical analysis of uranium-doped thorium dioxide: Introduction of a thoria force field with explicit polarization	AIP Advances	2015	5 (8)	87118	10.1063/1.4928438
lev	Atomic-Level Self-Assembly Mechanisms in p-Terphenyl-m-Dicarbonitrile on Ag(111) Surface	Phys. Chem. Chem. Phys.	2015	17	11182-11192	10.1039/c5cp00220f
lor	Atomistic Description of Pressure-Driven Flow of Aqueous Salt Solutions through Charged Silica Nanopores	J. Phys. Chem. C	2015	119 (22)	12298–12311	10.1021/jp5129639
lor	Solvation and Hydration of the Ceramide Headgroup in a Non-Polar Solution	J. Phys. Chem. B	2015	119 (1)	128-139	10.1021/jp5107789
mck	Atomic study of Fe3O3/SrTiO3 interface	Microsc. Microanal.	2015	21	1299	10.1017/S143192761500728X
mck	Electronic and magnetic properties of the cation vacancy defect in m-HfO2	Phys. Rev. B	2015	92	205124	10.1103/PhysRevB.92.205124
mck	Facet-Dependent Electron Trapping in TiO2 Nanocrystals	J. Phys. Chem. C	2015	119	1913	10.1021/jp511529u
mck	First principles modelling of electron tunneling between defects in m-HfO2	Microelectron. Eng.	2015	147	325	10.1016/j.mee.2015.04.009
mck	Relevance of non-equilibrium defect generation processes to resistive switching in TiO2	J. Appl. Phys.	2015	118	134103	10.1063/1.4932225
mck	Surface Specific Visible Light Luminescence from Composite Metal Oxide Nanocrystals	J. Mater. Sci.	2015	50	8153	10.1007/s10853-015-9393-2
mic	Enhancement of low-energy electron emission in 2D radioactive films	Nature Materials	2015	14	904	10.1038/NMAT4323
mic	Molecular simulations of heterogeneous ice nucleation. I. Controlling ice nucleation through surface hydrophilicity	J. Chem. Phys.	2015	142	184704	10.1063/1.4919714
mic	Molecular simulations of heterogeneous ice nucleation. II. Peeling back the layers	J. Chem. Phys.	2015	142	184705	10.1063/1.4919715
mic	The Many Faces of Heterogeneous Ice Nucleation: Interplay Between Surface Morphology and Hydrophobicity	J. Am. Chem. Soc.	2015	137	13658	10.1021/jacs.5b08748
muk	Computation of diffuse scattering arising from one-phonon excitations in a neutron time-of-flight single-crystal Laue diffraction experiment	J. App. Cryst.	2015	48	1122	10.1107/S1600576715010912
nat	Electronic Structure and Charge Transfer in the TiO2 Rutile (110)/Graphene Composite Using Hybrid DFT Calculations	J. Phys. Chem. C	2015	121 (8)	4158–4171	10.1021/acs.jpcc.6b12506
nic	Optical properties of alkali halide crystals from all-electron hybrid TD-DFT calculations	J. Chem. Phys.	2015	142	214705	10.1063/1.4921822
nic	Optimizing Oxygen Reduction Catalyst Morphologies from First Principles	J. Phys. Chem. C	2015	119 (29)	16804–16810	10.1021/acs.jpcc.5b05460
nic	Surface morphology of CuFeS2: The stability of the polar (112)/(-1-1-2) surfa10.1103/PhysRevB.92.155426ce pair	Phys. Rev. B	2015	92	155426	10.1103/PhysRevB.92.155426
par	A giant reconstruction of α-quartz (0001) interpreted as three domains of nano dauphine twins	Scientific Reports	2015	5	14545	10.1038/srep14545
par	Ab initio Investigation of the Layered Uranium Oxides U3O8 and U2O5	Dalton Trans.	2015	44	2613-2622	10.1039/C4DT02493A
par	Atomistic Investigation of the Structure and Transport Properties of Tilt Grain Boundaries of UO2	J. Nuc. Mater	2015	458	45-55	10.1016/j.jnucmat.2014.11.120
par	Computer Simulation of Defect Clusters in UO2 and their Dependence on Composition	J. Nuc. Mater	2015	456	329-333	10.1016/j.jnucmat.2014.10.001
par	Crystal Structure and Thermoelectric Properties of Sr–Mo Substituted CaMnO3: a Combined Experimental and Computational Study	J. Mater. Chem. C	2015	3	12245-12259	10.1039/C5TC02318A
par	Density Functional Theory Calculations of Defective UO2 at U3O7 stoichiometry	J. Nuc. Mater	2015	467	724-729	10.1016/j.jnucmat.2015.10.006
par	Hydride Ion Formation in Stoichiometric UO2	Chem. Commun.	2015	51	16209-16212	10.1039/C5CC04799D
par	Measuring the mechanical properties of molecular conformers	Nature Commun.	2015	5	8338	10.1038/ncomms9338
par	Measuring the mechanical properties of molecular conformers.	Nature Communications	2015	6	1	10.1038/ncomms9338
par	Modelling the effects of surfactant loading level on the sorption of organic contaminants on organoclays	RSC Adv.	2015	5 (58)	47022-47030	10.1039/C5RA05998D
par	Physisorption Controls the Conformation and Density of States of an Adsorbed Porphyrin	J. Phys. Chem. C	2015	just accepted	N/A	10.1021/acs.jpcc.5b08350
par	Tuning Thermoelectric Properties of Misfit Layered Cobaltites by Chemically Induced Strain	J. Phys. Chem. C	2015	119 (38)	21818–21827	10.1021/acs.jpcc.5b05583
per	Adatoms Underneath Single Porphyrin Molecules on Au(111)	J. Am. Chem. Soc.	2015	137	1844	10.1021/ja510528x
per	Toggling the local electric field with an embedded adatom switch	Nano Letters	2015	15	5564	DOI:10.1021/acs.nanolett.5b02145
per	Tunable magnetoresistance in an asymmetrically coupled single-molecule junction	Nature Nanotechnology	2015	10	259	10.1038/nnano.2014.326
roy	Charge-induced Dipole vs. Relativistically Enhanced Covalent Interactions in Ar-tagged Au-Ag Tetramers and Pentamers	J. Chem. Phys.	2015	143 (2)	24310	10.1063/1.4923255
roy	Messenger or Modifier? The Nature of Argon Bonds to Mixed Gold-Silver Trimers	Angew. Chem. Intl. Edn.	2015	54 (36)	10675-10680.	10.1002/anie.201503845
roy	O2 Dissociation on M@Pt Core-Shell Particles for 3d, 4d and 5d Transition Metals	J. Phys. Chem. C	2015	119 (20)	11031-11041	10.1021/jp511598e
roy	Optical Absorption Spectra and Structures of Ag6+ and Ag8+	Eur. Phys. J. D	2015	69 (6)	152	10.1140/epjd/e2015-60188-2
roy	Pool-BCGA: A Parallel Generation-Free Genetic Algorithm for the Ab Initio Global Optimisation of Nanoalloy Clusters	Phys. Chem. Chem. Phys.	2015	17 (3)	2104-2112	10.1039/c4cp04323e
roy	The Birmingham Parallel Genetic Algorithm and its Application to the Direct DFT Global Optimisation of IrN (N = 10-20) Clusters	Nanoscale	2015	7 (33)	14032-14038	10.1039/C5NR03774C
roy	The Effect of Dispersion Correction on the Adsorption of CO on Metallic Nanoparticles	J. Phys. Chem. A	2015	119 (37)	9703-9709	10.1021/acs.jpca.5b05710

sal	Are the Crystal Structures of Enantiopure and Racemic Mandelic Acids Determined by Kinetics or Thermodynamics?	J. Am. Chem. Soc.	2015	137 (34)	11095-11104	10.1021/jacs.5b05938
sal	Concomitant conformational dimorphism in 1,2-bis(9-anthryl)acetylene	CrystEngComm	2015	17(26)	4877-4882	10.1039/C5CE00745C
shl	Efficient Parameterization of Complex Molecule-Surface Force Field	J. Comput. Chem.	2015	36	1187-1195	10.1002/jcc.23904
shl	Hole trapping at hydrogenic defects in amorphous silicon dioxide	Microel. Eng.	2015	147	141-144	10.1016/j.mee.2015.04.073
shl	Hydrogen-Induced Rupture of Strained Si-O Bonds in Amorphous Silicon Dioxide	PRL	2015	114(11)	115503	10.1103/PhysRevLett.114.115503
shl	Identifying Performance Limiting Defects in Silicon Carbidepn-junctions: A Theoretical Study	Mater. Sci. Forum	2015	858	257-260	10.4028/www.scientific.net/MSF.858.257
shl	Modelling of oxygen vacancy aggregates in monoclinic HfO2: can they contribute to conductive filament formation?	J. Phys.: Condens. Matter	2015	27(41)	415401	10.1088/0953-8984/27/41/415401
shl	Optical signatures of intrinsic electron localization in amorphous SiO2	J. Phys.: Condens. Matter.	2015	27(26)	265501-6	10.1088/0953-8984/27/26/265501
shl	Photoinduced Br Desorption from CsBr Thin Films Grown on Cu (100)	J. Phys. Chem. C	2015	119(42)	24036-24045	10.1021/acs.jpcc.5b08275
shl	Theoretical models of hydrogen-induced defects in amorphous silicon dioxide	Phys. Rev. B	2015	92(1)	014107-11	10.1103/PhysRevB.92.014107
shu	Bond length effects during the dissociation of O2 on Ni(111)	Appl. Surf. Sci.	2015	346	329-334	10.1016/j.apsusc.2015.03.192
shu	Strategies for reducing basis set superposition error (BSSE) in O/Au and O/Ni	J. Phys. Chem. Solids	2015	86	19-26	10.1016/j.jpcs.2015.06.016
wal	A tunable amorphous p-type ternary oxide system: The highly mismatched alloy of copper tin oxide	J. Appl. Phys.	2015	118	105702	10.1063/1.4929752
wal	Ab Initio Molecular-Dynamics Simulation of Neuromorphic Computing in Phase-Change Memory Materials	Applied Materials & Interfaces	2015	<Just Accepted>	<Just Accepted>	10.1021/acsami.5b01825
wal	Absorbate-Induced Piezochromism in a Porous Molecular Crystal	Nano Lett.	2015	15	2149-2154	10.1021/acs.nanolett.5b00144
wal	Assessment of polyanion (BF4- and PF6-) substitutions in hybrid halide perovskites	J. Mater. Chem. A	2015	3	9067-9070	10.1039/c4ta05284f
wal	Band alignment of the hybrid halide perovskites CH 3 NH 3 PbCl 3, CH 3 NH 3 PbBr 3 and CH 3 NH 3 PbI 3	Mater. Horiz.	2015	Preprint	Preprint	10.1039/C4MH00174E
wal	Band energy control of molybdenum oxide by surface hydration	Appl. Phys. Lett.	2015	107	231605	10.1063/1.4937460
wal	Cation-Dependent Intrinsic Electrical Conductivity in Isostructural Tetrathiafulvalene-Based Microporous Metal–Organic Frameworks	J. Am. Chem. Soc.	2015	137	1774-1777	10.1021/ja512437u
wal	Chemical principles underpinning the performance of the metal–organic framework HKUST-1	Chem. Sci.	2015	6	3674-3683	10.1039/c5sc01489a
wal	Crystal structure optimisation using an auxiliary equation of state	J. Chem. Phys.	2015	143	184101	10.1063/1.4934716
wal	Crystalline adducts of the Lawsone molecule (2-hydroxy-1,4-naphthaquinone): optical properties and computational modelling	CrystEngComm	2015	17	7684	10.1039/C5CE01644D
wal	Electronic Excitations in Molecular Solids: Bridging Theory and Experiment	Faraday Discussions	2015	177	181-202	10.1039/C4FD00168K
wal	Energetics, thermal isomerisation and photochemistry of the linkage-isomer system [Ni(Et4dien)(η2-O,ON)(η1-NO2)]	CrystEngComm	2015	17	383-394	0.1039/C4CE01411A
wal	Ferroelectric materials for solar energy conversion: photoferroics revisited	Ener. Environ. Sci.	2015	Preprint	Preprint	10.1039/C4EE03523B
wal	Influence of the exchange-correlation functional on the quasi-harmonic lattice dynamics of II-VI semiconductors	J. Chem. Phys.	2015	143	64710	10.1063/1.4928058
wal	Magnetoelastic coupling in the cobalt adipate metal–organic framework from quasi-harmonic lattice dynamics	Journal of Materials Chemistry C	2015	3 (42)	11076-11080	10.1039/C5TC02633D
wal	Million-Fold Electrical Conductivity Enhancement in Fe2(DEBDC)versus Mn2(DEBDC) (E = S, O)	J. Am. Chem. Soc.	2015	137	6164-6167	10.1021/jacs.5b02897
wal	Modular design of SPIRO-OMeTAD analogues as hole transport materials in solar cells	Chem. Commun.	2015	51	8935-8938	10.1039/c5cc02129d
wal	Nanocrystals of Cesium Lead Halide Perovskites (CsPbX3, X = Cl, Br, and I): Novel Optoelectronic Materials Showing Bright Emission with Wide Color	Nano Lett.	2015	15	3692-3696	10.1021/nl5048779
wal	Phase stability and transformations in the halide perovskite CsSnI3	Phys. Rev. B	2015	91	144107	10.1103/PhysRevB.91.144107
wal	Photocatalytic Carbon Dioxide Reduction with Rhodium- based Catalysts in Solution and Heterogenized within Metal–Organic Frameworks	ChemSusChem	2015	8	603-608	10.1002/cssc.201403345
wal	Role of entropic effects in controlling the polymorphism in formate ABX 3 metal–organic frameworks	Chem. Comm.	2015	51	15538-15541	10.1039/C5CC06190C
wal	Solid-state chemistry of glassy antimony oxides	J. Mater. Chem. C	2015	3	11349	10.1039/C5TC02191J
wal	Vibrational spectra and lattice thermal conductivity of kesterite-structured Cu2ZnSnS4 and Cu2ZnSnSe	APL Materials	2015	3	41102	10.1063/1.4917044
wat	The electronic structure of sulvanite structured semiconductors Cu3MCh4 (M = V, Nb, Ta; Ch = S, Se, Te): prospects for optoelectronic applications.	J. Mater. Chem. C	2015	3	12236–12244	10.1039/c5tc02760h
wil	A density functional study of oxygen vacancy formation on α-Fe2O3(0001) surface and the effect of supported Au nanoparticles	Research on Chemical Intermediates	2015	41 (12)	9587-9601	10.1007/s11164-015-1984-7
wil	CO adsorption over Pd nanoparticles: A general framework for IR simulations on nanoparticles	Surf. Sci.	2015	in press	corrected proof	10.1016/j.susc.2015.07.014
wil	The functionalisation of graphite surfaces with nitric acid: identification of functional groups and their effects on gold deposition.	J. Catal.	2015	323	Oct-18	10.1016/j.jcat.2014.12.021
zwi	Chemical trends in the optical properties of rocksalt nanoparticles	Phys. Chem. Chem. Phys.	2015	17	28892-28900	10.1039/C5CP04851F
zwi	Modeling the Water Splitting Activity of a TiO2 Rutile Nanoparticle	J. Phys. Chem. C	2015	119	13384–13393	10.1021/acs.jpcc.5b01512
zwi	Tunable Organic Photocatalysts for Visible-Light-Driven HydrogenEvolution	J. Am. Chem. Soc.	2015	137	3265 – 3270	10.1021/ja511552k