Nora De Leeuw

List of Publications by Year in Descending Order

344 papers	11,051 citations	58 h-index	87 g-index
356 ext. papers	12,426 ext. citations	4.4 avg, IF	6.84 L-index

#	Paper	IF	Citations
344	A DFT Mechanistic Study on Base-Catalyzed Cleavage of the -O-4 Ether Linkage in Lignin: Implications for Selective Lignin Depolymerization.. *Frontiers in Chemistry*, **2022**, 10, 793759	5	
343	Understanding the Interactions between Triolein and Cosolvent Binary Mixtures Using Molecular Dynamics Simulations.. *ACS Omega*, **2022**, 7, 10212-10224	3.9	
342	Catalytic Reduction of Carbon Dioxide on the (001), (011), and (111) Surfaces of TiC and ZrC: A Computational Study.. *Journal of Physical Chemistry C*, **2022**, 126, 5138-5150	3.8	1
341	Photocatalytic Degradation of Rhodamine B Dye and Hydrogen Evolution by Hydrothermally Synthesized NaBH-Spiked ZnS Nanostructures.. *Frontiers in Chemistry*, **2022**, 10, 835832	5	0
340	Insights from density functional theory calculations into the effects of the adsorption and dissociation of water on the surface properties of zinc diphosphide (ZnP) nanocrystals. *Physical Chemistry Chemical Physics*, **2021**, 23, 26482-26493	3.6	0
339	Density Functional Theory Study of Ethylene Carbonate Adsorption on the (0001) Surface of Aluminum Oxide □AlO. *ACS Omega*, **2021**, 6, 29577-29587	3.9	0
338	Competitive adsorption geometries for the arsenate As(V) and phosphate P(V) oxyanions on magnetite surfaces: Experiments and theory. *American Mineralogist*, **2021**, 106, 374-388	2.9	4
337	First Steps towards Understanding the Non-Linear Impact of Mg on Calcite Solubility: A Molecular Dynamics Study. *Minerals (Basel, Switzerland)*, **2021**, 11, 407	2.4	2
336	Changes in CO2 Adsorption Affinity Related to Ni Doping in FeS Surfaces: A DFT-D3 Study. *Catalysts* , **2021**, 11, 486	4	2
335	Mechanism of Guaiacol Hydrodeoxygenation on Cu (111): Insights from Density Functional Theory Studies. *Catalysts*, **2021**, 11, 523	4	1
334	Behavior of S, SO, and SO on Pt (001), (011), and (111) surfaces: A DFT study. *Journal of Chemical Physics*, **2021**, 154, 194701	3.9	1
333	Combined Experimental and Theoretical Study of the Competitive Absorption of CO and NO by a Superbase Ionic Liquid. *ACS Sustainable Chemistry and Engineering*, **2021**, 9, 7578-7586	8.3	3
332	Catalytic Conversion of CO and H2 into Hydrocarbons on the Cobalt Co(111) Surface: Implications for the Fischer□ropsch Process. *Journal of Physical Chemistry C*, **2021**, 125, 11891-11903	3.8	3
331	A Perspective on Modelling Metallic Magnetic Nanoparticles in Biomedicine: From Monometals to Nanoalloys and Ligand-Protected Particles. *Materials*, **2021**, 14,	3.5	3
330	Predicting the Membrane Permeability of Fentanyl and Its Analogues by Molecular Dynamics Simulations. *Journal of Physical Chemistry B*, **2021**, 125, 8443-8449	3.4	2
329	TiO/CuO/CuO Multi-Nanolayers as Sensors for H and Volatile Organic Compounds: An Experimental and Theoretical Investigation. *ACS Applied Materials & Interfaces*, **2021**, 13, 32363-32380	9.5	9
328	CO reduction to acetic acid on the greigite FeS{111} surface. *Faraday Discussions*, **2021**, 229, 35-49	3.6	8

327	Quasielastic Neutron Scattering and Molecular Dynamics Simulation Study on the Molecular Behaviour of Catechol in Zeolite Beta. *Topics in Catalysis*, **2021**, 64, 707-721	2.3	0
326	Structural and dynamical properties of ionic liquids: a molecular dynamics study employing DL_POLY 4. *Molecular Simulation*, **2021**, 47, 152-160	2	2
325	The mechanism underlying the functionalisation of cobalt nanoparticles by carboxylic acids: a first-principles computational study. *Journal of Materials Chemistry B*, **2021**, 9, 4915-4928	7.3	2
324	Activating the FeS (001) Surface for CO2 Adsorption and Reduction through the Formation of Sulfur Vacancies: A DFT-D3 Study. *Catalysts*, **2021**, 11, 127	4	2
323	The role of surface oxidation and Fe-Ni synergy in Fe-Ni-S catalysts for CO hydrogenation. *Faraday Discussions*, **2021**, 230, 30-51	3.6	3
322	A surface oxidised Fe$_9$S$_8$ catalyst for the liquid phase hydrogenation of CO2. *Catalysis Science and Technology*, **2021**, 11, 779-784	5.5	6
321	Mercury exchange in zeolites Na-A and Na-Y studied by classical molecular dynamics simulations and ion exchange experiments. *Microporous and Mesoporous Materials*, **2021**, 315, 110903	5.3	2
320	Heterostructure-based devices with enhanced humidity stability for H2 gas sensing applications in breath tests and portable batteries. *Sensors and Actuators A: Physical*, **2021**, 329, 112804	3.9	4
319	Tailoring the selectivity of ultralow-power heterojunction gas sensors by noble metal nanoparticle functionalization. *Nano Energy*, **2021**, 88, 106241	17.1	5
318	How bulk and surface properties of TiSiC, VSiC, NbSiC and ZrSiC tune reactivity: a computational study. *Faraday Discussions*, **2021**, 230, 87-99	3.6	0
317	Effect of coverage on the magnetic properties of -COOH, -SH, and -NH ligand-protected cobalt nanoparticles. *Nanoscale*, **2021**, 13, 11844-11855	7.7	2
316	Lysine-arginine advanced glycation end-product cross-links and the effect on collagen structure: A molecular dynamics study. *Proteins: Structure, Function and Bioinformatics*, **2021**, 89, 521-530	4.2	3
315	Density Functional Theory Study of Monoclinic FeNbO4: Bulk Properties and Water Dissociation at the (010), (011), (110), and (111) Surfaces. *Journal of Physical Chemistry C*, **2021**, 125, 27566-27577	3.8	1
314	Surface functionalization of ZnO:Ag columnar thin films with AgAu and AgPt bimetallic alloy nanoparticles as an efficient pathway for highly sensitive gas discrimination and early hazard detection in batteries. *Journal of Materials Chemistry A*, **2020**, 8, 16246-16264	13	22
313	Atomistic Molecular Dynamics Simulations of Propofol and Fentanyl in Phosphatidylcholine Lipid Bilayers. *ACS Omega*, **2020**, 5, 14340-14353	3.9	8
312	Interaction of SO2 with the Platinum (001), (011), and (111) Surfaces: A DFT Study. *Catalysts*, **2020**, 10, 558	4	4
311	Electronic structure, ion diffusion and cation doping in the NaVO(PO) compound as a cathode material for Na-ion batteries. *Physical Chemistry Chemical Physics*, **2020**, 22, 6653-6659	3.6	10
310	Adsorbate-Induced Segregation of Cobalt from PtCo Nanoparticles: Modeling Au Doping and Core AuCo Alloying for the Improvement of Fuel Cell Cathode Catalysts. *Journal of Physical Chemistry C*, **2020**, 124, 18321-18334	3.8	4

309	Structural and Optical Properties of ZnO Thin Films Prepared by Molecular Precursor and Sol–Gel Methods. *Crystals*, **2020**, 10, 132	2.3	21
308	Towards a morphology of cobalt nanoparticles: size and strain effects. *Nanotechnology*, **2020**, 31, 195711	3.4	13
307	Ethylene carbonate adsorption on the major surfaces of lithium manganese oxide LiMnO spinel (0.000 Physical Chemistry Chemical Physics, **2020**, 22, 6763-6771	3.6	6
306	Exploring the formation of intrinsic p-type and n-type defects in CuO. *Physical Review Materials*, **2020**, 4,	3.2	9
305	Cu Electrodeposition on Nanostructured MoS2 and WS2 and Implications for HER Active Site Determination. *Journal of the Electrochemical Society*, **2020**, 167, 116517	3.9	2
304	Combined density functional theory and molecular dynamics study of SmACoMnO (A = Ca, Sr; x = 0.125, 0.25) cathode material for next generation solid oxide fuel cell. *Physical Chemistry Chemical Physics*, **2020**, 22, 692-699	3.6	6
303	Understanding the role of zinc dithiocarbamate complexes as single source precursors to ZnS nanomaterials. *Nanoscale Advances*, **2020**, 2, 798-807	5.1	7
302	Binding modes of carboxylic acids on cobalt nanoparticles. *Physical Chemistry Chemical Physics*, **2020**, 22, 985-996	3.6	12
301	Amino-functionalized MIL-101(Cr) photodegradation enhancement by sulfur-enriched copper sulfide nanoparticles: An experimental and DFT study. *Journal of Molecular Liquids*, **2020**, 319, 114341	6	15
300	Electronic Structure and Interface Energetics of CuBiO Photoelectrodes. *Journal of Physical Chemistry C*, **2020**, 124, 22416-22425	3.8	13
299	Nanostructured zeolite with brain-coral morphology and tailored acidity: a self-organized hierarchical porous material with MFI topology. *CrystEngComm*, **2020**, 22, 6275-6286	3.3	1
298	Electronic Excitations in Copper Oxides: Time-Dependent Density Functional Theory Calculations with a Self-Consistent Hybrid Kernel. *Journal of Physical Chemistry C*, **2020**, 124, 24995-25003	3.8	2
297	Influence of Topology and Brønsted Acid Site Presence on Methanol Diffusion in Zeolites Beta and MFI. *Catalysts*, **2020**, 10, 1342	4	6
296	A molecular dynamics study of the effect of water diffusion into bio-active phosphate-based glass surfaces on their dissolution behaviour. *Journal of Non-Crystalline Solids*, **2020**, 548, 120332	3.9	3
295	Interaction of hydrogen with actinide dioxide (011) surfaces. *Journal of Chemical Physics*, **2020**, 153, 014705	3.9	1
294	In silico studies of the interactions between propofol and fentanyl using Gaussian accelerated molecular dynamics. *Journal of Biomolecular Structure and Dynamics*, **2020**, 1-13	3.6	2
293	Single CuO/CuO/Cu Microwire Covered by a Nanowire Network as a Gas Sensor for the Detection of Battery Hazards. *ACS Applied Materials & Interfaces*, **2020**, 12, 42248-42263	9.5	17
292	Mechanisms of carbon dioxide reduction on strontium titanate perovskites. *Journal of Materials Chemistry A*, **2020**, 8, 9392-9398	13	12

291	Glucosepane is associated with changes to structural and physical properties of collagen fibrils. *Matrix Biology Plus*, **2019**, 4, 100013	5.1	5
290	Interaction of HO with the Platinum Pt (001), (011), and (111) Surfaces: A Density Functional Theory Study with Long-Range Dispersion Corrections. *Journal of Physical Chemistry C*, **2019**, 123, 27465-27476	3.8	20
289	Magnetic structure of UO and NpO by first-principle methods. *Physical Chemistry Chemical Physics*, **2019**, 21, 760-771	3.6	20
288	Density functional theory study explaining the underperformance of copper oxides as photovoltaic absorbers. *Physical Review B*, **2019**, 99,	3.3	23
287	Hydrogen adsorption on transition metal carbides: a DFT study. *Physical Chemistry Chemical Physics*, **2019**, 21, 5335-5343	3.6	25
286	A density functional theory study of the hydrogenation and reduction of the thio-spinel FeS{111} surface. *Physical Chemistry Chemical Physics*, **2019**, 21, 2426-2433	3.6	3
285	A DFT+U study of the oxidation of cobalt nanoparticles: Implications for biomedical applications. *Materialia*, **2019**, 7, 100381	3.2	18
284	Unraveling the Role of Lithium in Enhancing the Hydrogen Evolution Activity of MoS: Intercalation versus Adsorption. *ACS Energy Letters*, **2019**, 4, 1733-1740	20.1	25
283	Mixing thermodynamics and electronic structure of the Pt Ni (0 □1) bimetallic alloy.. *RSC Advances*, **2019**, 9, 16948-16954	3.7	4
282	Fe(II) and Fe(III) dithiocarbamate complexes as single source precursors to nanoscale iron sulfides: a combined synthetic and in situ XAS approach. *Nanoscale Advances*, **2019**, 1, 2965-2978	5.1	11
281	Carbon dioxide and water co-adsorption on the low-index surfaces of TiC, VC, ZrC and NbC: a DFT study. *Physical Chemistry Chemical Physics*, **2019**, 21, 10750-10760	3.6	13
280	Computational study of the mixed B-site perovskite SmBCoO (B = Mn, Fe, Ni, Cu) for next generation solid oxide fuel cell cathodes. *Physical Chemistry Chemical Physics*, **2019**, 21, 9407-9418	3.6	12
279	Advances in Sustainable Catalysis: A Computational Perspective. *Frontiers in Chemistry*, **2019**, 7, 182	5	27
278	Interaction of hydrogen with actinide dioxide (111) surfaces. *Journal of Chemical Physics*, **2019**, 150, 134701	3.3	4
277	Tautomerization of Phenol at the External Lewis Acid Sites of Scandium-, Iron- and Gallium-Substituted Zeolite MFI. *Journal of Physical Chemistry C*, **2019**, 123, 7604-7614	3.8	5
276	Liquid phase hydrogenation of CO2 to formate using palladium and ruthenium nanoparticles supported on molybdenum carbide. *New Journal of Chemistry*, **2019**, 43, 13985-13997	3.6	9
275	Mechanism of Photocatalytic Reduction of CO2 by Ag3PO4(111)/g-C3N4 Nanocomposite: A First-Principles Study. *Journal of Physical Chemistry C*, **2019**, 123, 22191-22201	3.8	21
274	The Origin of High Activity of Amorphous MoS in the Hydrogen Evolution Reaction. *ChemSusChem*, **2019**, 12, 4383-4389	8.3	54

273	Thermal Properties and Segregation Behavior of Pt Nanowires Modified with Au, Ag, and Pd Atoms: A Classical Molecular Dynamics Study. *Journal of Physical Chemistry C*, **2019**, 123, 20522-20531	3.8	1
272	Tuning ZnO Sensors Reactivity toward Volatile Organic Compounds via Ag Doping and Nanoparticle Functionalization. *ACS Applied Materials & Interfaces*, **2019**, 11, 31452-31466	9.5	43
271	First-principles DFT insights into the structural, elastic, and optoelectronic properties of □and □ZnP: implications for photovoltaic applications. *Journal of Physics Condensed Matter*, **2019**, 31, 265501	1.8	1
270	Reconsidering Calcium Dehydration as the Rate-Determining Step in Calcium Mineral Growth. *Journal of Physical Chemistry C*, **2019**, 123, 26895-26903	3.8	8
269	Modulation of the Ion Channel by Fentanyl: A Molecular Dynamics Study. *Biochemistry*, **2019**, 58, 4804-4808	3.0	6
268	The Origin of High Activity of Amorphous MoS2 in the Hydrogen Evolution Reaction. *ChemSusChem*, **2019**, 12, 4336-4336	8.3	1
267	Tuning the electronic band gap of Cu2O via transition metal doping for improved photovoltaic applications. *Physical Review Materials*, **2019**, 3,	3.2	8
266	Hydrazine adsorption on perfect and defective fcc nickel (100), (110) and (111) surfaces: A dispersion corrected DFT-D2 study. *Applied Surface Science*, **2019**, 480, 1014-1024	6.7	9
265	Enhancing the electrocatalytic activity of 2H-WS for hydrogen evolution via defect engineering. *Physical Chemistry Chemical Physics*, **2019**, 21, 6071-6079	3.6	35
264	Dependence of electron transfer dynamics on the number of graphene layers in □stacked 2D materials: insights from ab initio nonadiabatic molecular dynamics. *Physical Chemistry Chemical Physics*, **2019**, 21, 23198-23208	3.6	6
263	Molecular behaviour of phenol in zeolite Beta catalysts as a function of acid site presence: a quasielastic neutron scattering and molecular dynamics simulation study. *Catalysis Science and Technology*, **2019**, 9, 6700-6713	5.5	9
262	Noncollinear Relativistic DFT + U Calculations of Actinide Dioxide Surfaces. *Journal of Physical Chemistry C*, **2019**, 123, 356-366	3.8	11
261	Relative orientation of collagen molecules within a fibril: a homology model for homo sapiens type I collagen. *Journal of Biomolecular Structure and Dynamics*, **2019**, 37, 537-549	3.6	5
260	Bulk and surface properties of metal carbides: implications for catalysis. *Physical Chemistry Chemical Physics*, **2018**, 20, 6905-6916	3.6	53
259	Stability and mobility of supported Ni (n□= 1-10) clusters on ZrO(111) and YSZ(111) surfaces: a density functional theory study. *Faraday Discussions*, **2018**, 208, 87-104	3.6	6
258	Modelling water diffusion in plasticizers: development and optimization of a force field for 2,4-dinitroethylbenzene and 2,4,6-trinitroethylbenzene.. *RSC Advances*, **2018**, 8, 5728-5739	3.7	0
257	Ab initio investigation of the thermodynamics of cation distribution and of the electronic and magnetic structures in the LiMn2O4 spinel. *Physical Review B*, **2018**, 97,	3.3	17
256	Effect on the mechanical properties of type I collagen of intra-molecular lysine-arginine derived advanced glycation end-product cross-linking. *Journal of Biomechanics*, **2018**, 67, 55-61	2.9	16

255	Calcium Phosphate Deposition on Planar and Stepped (101) Surfaces of Anatase TiO: Introducing an Interatomic Potential for the TiO/Ca-PO/Water Interface. *Langmuir*, **2018**, 34, 10144-10152	4	3
254	Hidden magnetic order in plutonium dioxide nuclear fuel. *Physical Chemistry Chemical Physics*, **2018**, 20, 20943-20951	3.6	20
253	CO2 and H2 Adsorption and Reaction at Nin/YSZ(111) Interfaces: A Density Functional Theory Study. *Journal of Physical Chemistry C*, **2018**, 122, 19463-19472	3.8	11
252	CO interaction with violarite (FeNiS) surfaces: a dispersion-corrected DFT study. *Physical Chemistry Chemical Physics*, **2018**, 20, 20439-20446	3.6	13
251	Insight into the Nature of Iron Sulfide Surfaces During the Electrochemical Hydrogen Evolution and CO Reduction Reactions. *ACS Applied Materials & Interfaces*, **2018**, 10, 32078-32085	9.5	21
250	A highly reactive precursor in the iron sulfide system. *Nature Communications*, **2018**, 9, 3125	17.4	52
249	Theory as a driving force to understand reactions on nanoparticles: general discussion. *Faraday Discussions*, **2018**, 208, 147-185	3.6	1
248	Initial Oxygen Incorporation in the Prismatic Surfaces of Troilite FeS. *Journal of Physical Chemistry C* , **2018**, 122, 12810-12818	3.8	13
247	Reactivity of CO on the surfaces of magnetite (FeO), greigite (FeS) and mackinawite (FeS). *Philosophical Transactions Series A, Mathematical, Physical, and Engineering Sciences*, **2018**, 376,	3	18
246	Adsorption and Desulfurization Mechanism of Thiophene on Layered FeS(001), (011), and (111) Surfaces: A Dispersion-Corrected Density Functional Theory Study. *Journal of Physical Chemistry C*, **2018**, 122, 359-370	3.8	11
245	Tuning doping and surface functionalization of columnar oxide films for volatile organic compound sensing: experiments and theory. *Journal of Materials Chemistry A*, **2018**, 6, 23669-23682	13	27
244	Ab initio investigation of O adsorption on Ca-doped LaMnO cathodes in solid oxide fuel cells. *Physical Chemistry Chemical Physics*, **2018**, 20, 28685-28698	3.6	7
243	A molecular dynamics study of plasticiser migration in nitrocellulose binders. *New Journal of Chemistry*, **2018**, 42, 17420-17428	3.6	4
242	Computational Study of NaVOPO4 Polymorphs as Cathode Materials for Na-Ion Batteries: Diffusion, Electronic Properties, and Cation-Doping Behavior. *Journal of Physical Chemistry C*, **2018**, 122, 25829-25836	3.8	24
241	Persistent Quantum Coherence and Strong Coupling Enable Fast Electron Transfer across the CdS/TiO2 Interface: A Time-Domain ab Initio Simulation. *Journal of Physical Chemistry C*, **2018**, 122, 25606-25616	3.8	12
240	Density functional theory characterization of the structures of HAsO and HAsO adsorption complexes on ferrihydrite. *Environmental Sciences: Processes and Impacts*, **2018**, 20, 977-987	4.3	14
239	Mapping intermolecular interactions and active site conformations: from human MMP-1 crystal structure to molecular dynamics free energy calculations. *Journal of Biomolecular Structure and Dynamics*, **2017**, 35, 564-573	3.6	11
238	Computational study of glucosepane-water and hydrogen bond formation: an electron topology and orbital analysis. *Journal of Biomolecular Structure and Dynamics*, **2017**, 35, 1127-1137	3.6	5

237	Enhanced UV and ethanol vapour sensing of a single 3-D ZnO tetrapod alloyed with Fe2O3 nanoparticles. *Sensors and Actuators B: Chemical*, **2017**, 245, 448-461	8.5	39
236	Hybridization of Zinc Oxide Tetrapods for Selective Gas Sensing Applications. *ACS Applied Materials & Interfaces*, **2017**, 9, 4084-4099	9.5	110
235	A DFT+U investigation of hydrogen adsorption on the LaFeO(010) surface. *Physical Chemistry Chemical Physics*, **2017**, 19, 7399-7409	3.6	22
234	Structures and Properties of As(OH) Adsorption Complexes on Hydrated Mackinawite (FeS) Surfaces: A DFT-D2 Study. *Environmental Science & Technology*, **2017**, 51, 3461-3470	10.3	34
233	Nanosensors: Multifunctional Materials: A Case Study of the Effects of Metal Doping on ZnO Tetrapods with Bismuth and Tin Oxides (Adv. Funct. Mater. 6/2017). *Advanced Functional Materials*, **2017**, 27,	15.6	1
232	Transport properties of water molecules confined between hydroxyapaptite surfaces: A Molecular dynamics simulation approach. *Applied Surface Science*, **2017**, 418, 296-301	6.7	19
231	Selective hydrogenation of CO on FeS{111}: a computational study. *Faraday Discussions*, **2017**, 197, 325-336	3.6	5
230	Modeling of complex interfaces: Gadolinium-doped ceria in contact with yttria-stabilized zirconia. *Journal of the American Ceramic Society*, **2017**, 100, 3329-3339	3.8	7
229	Catalysis for Fuels: general discussion. *Faraday Discussions*, **2017**, 197, 165-205	3.6	4
228	Synthesis, Crystal Structures, and Properties of Zeolite-Like T3(H3O)2[M(CN)6]2□H2O (T = Co, Zn; M = Ru, Os). *European Journal of Inorganic Chemistry*, **2017**, 2017, 2980-2989	2.3	9
227	Effect of strontium inclusion on the bioactivity of phosphate-based glasses. *Journal of Materials Science*, **2017**, 52, 9014-9022	4.3	12
226	Density functional theory study of the zeolite-mediated tautomerization of phenol and catechol. *Molecular Catalysis*, **2017**, 433, 334-345	3.3	13
225	A computational study of the electronic properties, ionic conduction, and thermal expansion of SmACoO and SmACoO (A = Ba, Ca, Sr, and x = 0.25, 0.5) as intermediate temperature SOFC cathodes. *Physical Chemistry Chemical Physics*, **2017**, 19, 13960-13969	3.6	14
224	A kinetic model of water adsorption, clustering and dissociation on the FeS{001} surface. *Physical Chemistry Chemical Physics*, **2017**, 19, 12045-12055	3.6	14
223	Effect of nickel monolayer deposition on the structural and electronic properties of the low miller indices of (bcc) iron: A DFT study. *Applied Surface Science*, **2017**, 400, 293-303	6.7	8
222	Multifunctional Materials: A Case Study of the Effects of Metal Doping on ZnO Tetrapods with Bismuth and Tin Oxides. *Advanced Functional Materials*, **2017**, 27, 1604676	15.6	101
221	Density Functional Theory Study of Ni Clusters Supported on the ZrO2(111) Surface. *Fuel Cells*, **2017**, 17, 125-131	2.9	13
220	Micro-kinetic simulations of the catalytic decomposition of hydrazine on the Cu(111) surface. *Faraday Discussions*, **2017**, 197, 41-57	3.6	13

219	Combining nano-physical and computational investigations to understand the nature of "aging" in dermal collagen. *International Journal of Nanomedicine*, **2017**, 12, 3303-3314	7.3	10
218	Periodic DFT+U investigation of the bulk and surface properties of marcasite (FeS). *Physical Chemistry Chemical Physics*, **2017**, 19, 27478-27488	3.6	21
217	Structures and properties of phosphate-based bioactive glasses from computer simulation: a review. *Journal of Materials Chemistry B*, **2017**, 5, 5297-5306	7.3	9
216	Detection of Posner's clusters during calcium phosphate nucleation: a molecular dynamics study. *Journal of Materials Chemistry B*, **2017**, 5, 7274-7284	7.3	36
215	Phase stability and thermodynamic properties of FeS polymorphs. *Journal of Physics and Chemistry of Solids*, **2017**, 111, 317-323	3.9	6
214	Anisotropic diffusion of water molecules in hydroxyapatite nanopores. *Physics and Chemistry of Minerals*, **2017**, 44, 509-519	1.6	9
213	CO activation and dissociation on the low miller index surfaces of pure and Ni-coated iron metal: a DFT study. *Physical Chemistry Chemical Physics*, **2017**, 19, 19478-19486	3.6	9
212	Periodic modeling of zeolite Ti-LTA. *Journal of Chemical Physics*, **2017**, 147, 074701	3.9	6
211	Molecular Dynamics Simulations of Hydroxyapatite Nanopores in Contact with Electrolyte Solutions: The Effect of Nanoconfinement and Solvated Ions on the Surface Reactivity and the Structural, Dynamical, and Vibrational Properties of Water. *Crystals*, **2017**, 7, 57	2.3	16
210	DFT+U study of the structures and properties of the actinide dioxides. *Journal of Nuclear Materials*, **2017**, 492, 269-278	3.3	60
209	ForceGen: atomic covalent bond value derivation for Gromacs. *Journal of Molecular Modeling*, **2017**, 24, 5	2	10
208	DFT-D2 Study of the Adsorption and Dissociation of Water on Clean and Oxygen-Covered {001} and {011} Surfaces of Mackinawite (FeS). *Journal of Physical Chemistry C*, **2016**, 120, 21441-21450	3.8	26
207	Enhanced Photoresponse of FeS Films: The Role of Marcasite-Pyrite Phase Junctions. *Advanced Materials*, **2016**, 28, 9602-9607	24	53
206	Intra-molecular lysine-arginine derived advanced glycation end-product cross-linking in Type I collagen: A molecular dynamics simulation study. *Biophysical Chemistry*, **2016**, 218, 42-46	3.5	11
205	Molecular dynamics simulations of bio-active phosphate-based glass surfaces. *Journal of Non-Crystalline Solids*, **2016**, 451, 131-137	3.9	7
204	Combined EXAFS, XRD, DRIFTS, and DFT Study of Nano Copper-Based Catalysts for CO2 Hydrogenation. *ACS Catalysis*, **2016**, 6, 5823-5833	13.1	35
203	A force field for mackinawite surface simulations in an aqueous environment. *Theoretical Chemistry Accounts*, **2016**, 135, 1	1.9	4
202	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. *Surface Science*, **2016**, 653, 153-162	1.8	14

201	Investigating structural features which control the dissolution of bioactive phosphate glasses: Beyond the network connectivity. *Journal of Non-Crystalline Solids*, **2016**, 432, 31-34	3.9	32
200	Methanol formation from CO2 catalyzed by Fe3S4{111}: formate versus hydrocarboxyl pathways. *Faraday Discussions*, **2016**, 188, 161-80	3.6	25
199	A density functional theory study of arsenic immobilization by the Al(III)-modified zeolite clinoptilolite. *Physical Chemistry Chemical Physics*, **2016**, 18, 11297-305	3.6	7
198	A density functional theory study of uranium-doped thoria and uranium adatoms on the major surfaces of thorium dioxide. *Journal of Nuclear Materials*, **2016**, 473, 99-111	3.3	20
197	A density functional theory study of the structure of pure-silica and aluminium-substituted MFI nanosheets. *Journal of Solid State Chemistry*, **2016**, 237, 192-203	3.3	21
196	CuO Surfaces and CO2 Activation: A Dispersion-Corrected DFT+U Study. *Journal of Physical Chemistry C*, **2016**, 120, 2198-2214	3.8	109
195	Structure and dynamics of water at the mackinawite (001) surface. *Journal of Chemical Physics*, **2016**, 144, 094706	3.9	12
194	Publisher's Note: "Ab initio study of vacancy formation in cubic LaMnO and SmCoO as cathode materials in solid oxide fuel cells" [J. Chem. Phys. 145, 014703 (2016)]. *Journal of Chemical Physics*, **2016**, 145, 199901	3.9	2
193	A DFT+U study of the structural, electronic, magnetic, and mechanical properties of cubic and orthorhombic SmCoO. *Journal of Chemical Physics*, **2016**, 145, 224704	3.9	10
192	DFT-D2 simulations of water adsorption and dissociation on the low-index surfaces of mackinawite (FeS). *Journal of Chemical Physics*, **2016**, 144, 174704	3.9	23
191	A density functional theory study of the adsorption behaviour of CO2 on Cu2O surfaces. *Journal of Chemical Physics*, **2016**, 145, 044709	3.9	43
190	Ab initio study of vacancy formation in cubic LaMnO3 and SmCoO3 as cathode materials in solid oxide fuel cells. *Journal of Chemical Physics*, **2016**, 145, 014703	3.9	20
189	Catalytic water dissociation by greigite FeS surfaces: density functional theory study. *Proceedings of the Royal Society A: Mathematical, Physical and Engineering Sciences*, **2016**, 472, 20160080	2.4	14
188	Early Oxidation Processes on the Greigite Fe3S4(001) Surface by Water: A Density Functional Theory Study. *Journal of Physical Chemistry C*, **2016**, 120, 8616-8629	3.8	26
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