Nora De Leeuw

List of Publications by Citations

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	Surface Structure and Morphology of Calcium Carbonate Polymorphs Calcite, Aragonite, and Vaterite: An Atomistic Approach. *Journal of Physical Chemistry B*, **1998**, 102, 2914-2922	3.4	402
343	Atomistic simulation of dislocations, surfaces and interfaces in MgO. *Journal of the Chemical Society, Faraday Transactions*, **1996**, 92, 433		374
342	Magnesium incorporation into hydroxyapatite. *Biomaterials*, **2011**, 32, 1826-37	15.6	245
341	Modeling the Surface Structure and Stability of □Quartz. *Journal of Physical Chemistry B*, **1999**, 103, 1270-1277	3.4	181
340	Molecular-dynamics simulation of MgO surfaces in liquid water using a shell-model potential for water. *Physical Review B*, **1998**, 58, 13901-13908	3.3	175
339	Atomistic simulation of the effect of molecular adsorption ofwater on the surface structure and energies of calcitesurfaces. *Journal of the Chemical Society, Faraday Transactions*, **1997**, 93, 467-475		172
338	Bio-inspired CO2 conversion by iron sulfide catalysts under sustainable conditions. *Chemical Communications*, **2015**, 51, 7501-4	5.8	149
337	Symmetry-adapted configurational modelling of fractional site occupancy in solids. *Journal of Physics Condensed Matter*, **2007**, 19, 256201	1.8	146
336	The Structure of Bioactive Silicate Glasses: New Insight from Molecular Dynamics Simulations. *Chemistry of Materials*, **2007**, 19, 95-103	9.6	140
335	Vacancy ordering and electronic structure of □FeO□(maghemite): a theoretical investigation. *Journal of Physics Condensed Matter*, **2010**, 22, 255401	1.8	137
334	Shell-model molecular dynamics calculations of modified silicate glasses. *Physical Review B*, **2006**, 73,	3.3	136
333	A DFT study of the structures, stabilities and redox behaviour of the major surfaces of magnetite Fe□O□ *Physical Chemistry Chemical Physics*, **2014**, 16, 21082-97	3.6	135
332	Atomistic Simulation of the Effect of Dissociative Adsorption of Water on the Surface Structure and Stability of Calcium and Magnesium Oxide. *The Journal of Physical Chemistry*, **1995**, 99, 17219-17225		131
331	A computer modelling study of the uptake, structure and distribution of carbonate defects in hydroxy-apatite. *Biomaterials*, **2006**, 27, 2150-61	15.6	129
330	Synthesis, characterization and DFT studies of zinc-doped copper oxide nanocrystals for gas sensing applications. *Journal of Materials Chemistry A*, **2016**, 4, 6527-6539	13	119
329	Hybridization of Zinc Oxide Tetrapods for Selective Gas Sensing Applications. *ACS Applied Materials & Interfaces*, **2017**, 9, 4084-4099	9.5	110
328	Reduction of Carbon Dioxide to Formate at Low Overpotential Using a Superbase Ionic Liquid. *Angewandte Chemie - International Edition*, **2015**, 54, 14164-8	16.4	110

327	CuO Surfaces and CO2 Activation: A Dispersion-Corrected DFT+U Study. *Journal of Physical Chemistry C*, **2016**, 120, 2198-2214	3.8	109
326	Density functional theory study of the binding of glycine, proline, and hydroxyproline to the hydroxyapatite (0001) and (0110) surfaces. *Langmuir*, **2009**, 25, 5018-25	4	109
325	Computer simulations of the adsorption of citric acid at hydroxyapatite surfaces. *Journal of Crystal Growth*, **2006**, 294, 60-68	1.6	104
324	Molecular Dynamics Simulations of the Growth Inhibiting Effect of Fe2+, Mg2+, Cd2+, and Sr2+ on Calcite Crystal Growth. *Journal of Physical Chemistry B*, **2002**, 106, 5241-5249	3.4	102
323	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
322	A computer modelling study of the effect of water on the surface structure and morphology of fluorapatite: introducing a Ca10(PO4)6F2 potential model. *Journal of Materials Chemistry*, **2002**, 12, 2633-2642		98
321	Surface simulation studies of the hydration of white rust Fe(OH)2, goethite □FeO(OH) and hematite □Fe2O3. *Geochimica Et Cosmochimica Acta*, **2007**, 71, 1655-1673	5.5	93
320	Modelling the effect of water on the surface structure and stability of forsterite. *Physics and Chemistry of Minerals*, **2000**, 27, 332-341	1.6	93
319	A computational study of the surface structure and reactivity of calcium fluoride. *Journal of Materials Chemistry*, **2003**, 13, 93-101		86
318	A computer modelling study of the uptake and segregation of fluoride ions at the hydrated hydroxyapatite (0001) surface: introducing a Ca10(PO4)6(OH)2 potential model. *Physical Chemistry Chemical Physics*, **2004**, 6, 1860-1866	3.6	84
317	A Computer Modeling Study of the Inhibiting Effect of Organic Adsorbates on Calcite Crystal Growth. *Crystal Growth and Design*, **2004**, 4, 123-133	3.5	84
316	Structure and dynamics of the hydrated magnesium ion and of the solvated magnesium carbonates: insights from first principles simulations. *Physical Chemistry Chemical Physics*, **2010**, 12, 894-901	3.6	83
315	Molecular dynamics simulations of the interaction of citric acid with the hydroxyapatite (0001) and (01$\bar{1}$0) surfaces in an aqueous environment. *CrystEngComm*, **2007**, 9, 1178	3.3	83
314	Calcite surface structure and reactivity: molecular dynamics simulations and macroscopic surface modelling of the calcite-water interface. *Physical Chemistry Chemical Physics*, **2012**, 14, 15145-57	3.6	82
313	Origin of water in the inner Solar System: A kinetic Monte Carlo study of water adsorption on forsterite. *Icarus*, **2008**, 198, 400-407	3.8	80
312	Modeling the Competitive Adsorption of Water and Methanoic Acid on Calcite and Fluorite Surfaces. *Langmuir*, **1998**, 14, 5900-5906	4	80
311	Molecular dynamics simulation of crystal dissolution from calcite steps. *Physical Review B*, **1999**, 60, 13792-13799	3.3	80
310	Resisting the Onset of Hydroxyapatite Dissolution through the Incorporation of Fluoride. *Journal of Physical Chemistry B*, **2004**, 108, 1809-1811	3.4	79

309	Electronic charge transfer between ceria surfaces and gold adatoms: a GGA+U investigation. *Physical Chemistry Chemical Physics*, **2009**, 11, 5246-52	3.6	78
308	A Density Functional Theory Study of the Adsorption of Benzene on Hematite (□Fe2O3) Surfaces. *Minerals (Basel, Switzerland)*, **2014**, 4, 89-115	2.4	77
307	Density functional theory calculations of adsorption of water at calcium oxide and calcium fluoride surfaces. *Surface Science*, **2000**, 452, 9-19	1.8	75
306	Modelling the effect of water on cation exchange in zeolite A. *Journal of Materials Chemistry*, **2002**, 12, 124-131		73
305	Local ordering of hydroxy groups in hydroxyapatite. *Chemical Communications*, **2001**, 1646-7	5.8	72
304	Active Nature of Primary Amines during Thermal Decomposition of Nickel Dithiocarbamates to Nickel Sulfide Nanoparticles. *Chemistry of Materials*, **2014**, 26, 6281-6292	9.6	70
303	Adsorption of hydrazine on the perfect and defective copper (111) surface: A dispersion-corrected DFT study. *Surface Science*, **2014**, 622, 1-8	1.8	68
302	Molecular Dynamics Simulation of the Early Stages of Nucleation of Hydroxyapatite at a Collagen Template. *Crystal Growth and Design*, **2012**, 12, 756-763	3.5	66
301	A density functional theory study of the interaction of collagen peptides with hydroxyapatite surfaces. *Langmuir*, **2010**, 26, 14535-42	4	66
300	Modeling the Surface Structure and Reactivity of Pyrite:□Introducing a Potential Model for FeS2. *Journal of Physical Chemistry B*, **2000**, 104, 7969-7976	3.4	64
299	A comparative DFT study of the mechanical and electronic properties of greigite Fe3S4 and magnetite Fe3O4. *Journal of Chemical Physics*, **2013**, 138, 204712	3.9	63
298	A computer modeling study of the competitive adsorption of water and organic surfactants at surfaces of the mineral scheelite. *Langmuir*, **2004**, 20, 3984-94	4	63
297	Surface□water interactions in the dolomite problem. *Physical Chemistry Chemical Physics*, **2001**, 3, 3217-3221	3.6	63
296	Computer simulations of water interactions with low-coordinated forsterite surface sites: Implications for the origin of water in the inner solar system. *Earth and Planetary Science Letters*, **2010**, 300, 11-18	5.3	62
295	Structural and electronic properties of modified sodium and soda-lime silicate glasses by Car□Parrinello molecular dynamics. *Journal of Materials Chemistry*, **2006**, 16, 1950-1955		62
294	Combined Density Functional Theory and Interatomic Potential Study of the Bulk and Surface Structures and Properties of the Iron Sulfide Mackinawite (FeS). *Journal of Physical Chemistry C*, **2008**, 112, 10960-10967	3.8	60
293	Atomistic simulation of oxide surfaces and their reactivity with water. *Faraday Discussions*, **1999**, 114, 381-393	3.6	60
292	DFT+U study of the structures and properties of the actinide dioxides. *Journal of Nuclear Materials*, **2017**, 492, 269-278	3.3	60

291	First-principles study of the inversion thermodynamics and electronic structure of FeM2X4 (thio)spinels (M=Cr, Mn, Co, Ni; X=O, S). *Physical Review B*, **2015**, 91,	3.3	59
290	Redox Behavior of the Model Catalyst Pd/CeO2/Pt(111). *Journal of Physical Chemistry C*, **2008**, 112, 10918-10922	3.8	59
289	A computational investigation of stoichiometric and calcium-deficient oxy- and hydroxy-apatites. *Faraday Discussions*, **2007**, 134, 195-214; discussion 215-33, 415-9	3.6	59
288	Computer simulations of structures and properties of the biomaterial hydroxyapatite. *Journal of Materials Chemistry*, **2010**, 20, 5376		58
287	On the difficulties of present theoretical models to predict the oxidation state of atomic Au adsorbed on regular sites of CeO2(111). *Journal of Chemical Physics*, **2009**, 131, 094702	3.9	58
286	Ab initio molecular dynamics study of 45S5 bioactive silicate glass. *Journal of Physical Chemistry B*, **2006**, 110, 25810-6	3.4	57
285	An Ångström-sized window on the origin of water in the inner solar system: Atomistic simulation of adsorption of water on olivine. *Journal of Crystal Growth*, **2006**, 294, 83-95	1.6	57
284	A combined density functional theory and interatomic potential-based simulation study of the hydration of nano-particulate silicate surfaces. *Surface Science*, **2004**, 554, 193-210	1.8	56
283	Density functional theory calculations of local ordering of hydroxy groups and fluoride ions in hydroxyapatite. *Physical Chemistry Chemical Physics*, **2002**, 4, 3865-3871	3.6	56
282	The Origin of High Activity of Amorphous MoS in the Hydrogen Evolution Reaction. *ChemSusChem*, **2019**, 12, 4383-4389	8.3	54
281	Theoretical Investigation of the Deposition of Cu, Ag, and Au Atoms on the ZrO2(111) Surface. *Journal of Physical Chemistry C*, **2007**, 111, 10448-10454	3.8	54
280	Bulk and surface properties of metal carbides: implications for catalysis. *Physical Chemistry Chemical Physics*, **2018**, 20, 6905-6916	3.6	53
279	Enhanced Photoresponse of FeS Films: The Role of Marcasite-Pyrite Phase Junctions. *Advanced Materials*, **2016**, 28, 9602-9607	24	53
278	Effect of Chemisorption and Physisorption of Water on the Surface Structure and Stability of alpha-Alumina. *Journal of the American Ceramic Society*, **2004**, 82, 3209-2316	3.8	53
277	A combined ab initio and atomistic simulation study of the surface and interfacial structures and energies of hydrated scheelite: introducing a CaWO4 potential model. *Surface Science*, **2003**, 531, 159-176	1.8	53
276	A highly reactive precursor in the iron sulfide system. *Nature Communications*, **2018**, 9, 3125	17.4	52
275	Electronic and magnetic structure of Fe3S4: GGA+U investigation. *Physical Review B*, **2009**, 79,	3.3	52
274	Phase control during the synthesis of nickel sulfide nanoparticles from dithiocarbamate precursors. *Nanoscale*, **2016**, 8, 11067-75	7.7	52

273	Computer Modeling Study of the Effect of Hydration on the Stability of a Silica Nanotube. *Nano Letters*, **2003**, 3, 1347-1352	11.5	51
272	Density Functional Theory Calculations of Hydrogen-Containing Defects in Forsterite, Periclase, and □Quartz. *Journal of Physical Chemistry B*, **2001**, 105, 9747-9754	3.4	50
271	CO2 Capture in Wet and Dry Superbase Ionic Liquids. *Journal of Solution Chemistry*, **2015**, 44, 511-527	1.8	49
270	Molecular dynamics simulations of hydration, dissolution and nucleation processes at the alpha-quartz (0001) surface in liquid water. *Dalton Transactions*, **2006**, 2623-34	4.3	49
269	Density Functional Theory Study of the Adsorption of Hydrazine on the Perfect and Defective Copper (100), (110), and (111) Surfaces. *Journal of Physical Chemistry C*, **2014**, 118, 26103-26114	3.8	48
268	Modelling the effects of salt solutions on the hydration of calcium ions. *Physical Chemistry Chemical Physics*, **2014**, 16, 7772-85	3.6	46
267	The onset of calcium carbonate nucleation: a density functional theory molecular dynamics and hybrid microsolvation/continuum study. *Journal of Physical Chemistry B*, **2008**, 112, 6965-75	3.4	46
266	Modeling absorption and segregation of magnesium and cadmium ions to calcite surfaces: Introducing MgCO3 and CdCO3 potential models. *Journal of Chemical Physics*, **2000**, 112, 4326-4333	3.9	46
265	Atomistic simulation of adsorption of water on three-, four- and five-coordinated surface sites of magnesium oxide. *Journal of the Chemical Society, Faraday Transactions*, **1996**, 92, 2081		45
264	Interatomic potential models for natural apatite crystals: incorporating strontium and the lanthanides. *Journal of Computational Chemistry*, **2006**, 27, 253-66	3.5	44
263	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
262	He incorporation and diffusion pathways in pure and defective zircon ZrSiO4: A density functional theory study. *Chemical Geology*, **2009**, 258, 182-196	4.2	43
261	A theoretical investigation of alpha-Fe2O3-Cr2O3 solid solutions. *Physical Chemistry Chemical Physics*, **2009**, 11, 808-15	3.6	43
260	A density functional theory study of the adsorption behaviour of CO2 on Cu2O surfaces. *Journal of Chemical Physics*, **2016**, 145, 044709	3.9	43
259	First Principles Simulations of the Structural and Dynamical Properties of Hydrated Metal Ions Me2+ and Solvated Metal Carbonates (Me = Ca, Mg, and Sr). *Crystal Growth and Design*, **2010**, 10, 4292-4302	3.5	41
258	Activation and dissociation of CO2 on the (001), (011), and (111) surfaces of mackinawite (FeS): A dispersion-corrected DFT study. *Journal of Chemical Physics*, **2015**, 143, 094703	3.9	40
257	The formation of nanoscale structures in soluble phosphosilicate glasses for biomedical applications: MD simulations. *Faraday Discussions*, **2007**, 136, 45-55; discussion 107-23	3.6	40
256	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

255	Cation distribution and magnetic ordering in FeSbO4. *Journal of Materials Chemistry*, **2003**, 13, 2848		39
254	Adsorption of methylamine on mackinawite (FES) surfaces: a density functional theory study. *Journal of Chemical Physics*, **2013**, 139, 124708	3.9	38
253	Density Functional Theory Calculations of the Interaction of Hydrazine with Low-Index Copper Surfaces. *Journal of Physical Chemistry C*, **2009**, 113, 15714-15722	3.8	38
252	Electronic structure and magnetic coupling in FeSbO4: A DFT study using hybrid functionals and GGA+U methods. *Physical Review B*, **2006**, 73,	3.3	37
251	Catalytic Dissociation of Water on the (001), (011), and (111) Surfaces of Violarite, FeNi2S4: A DFT-D2 Study. *Journal of Physical Chemistry C*, **2014**, 118, 1958-1967	3.8	36
250	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
249	Proton-containing defects at forsterite {010} tilt grain boundaries and stepped surfaces. *American Mineralogist*, **2000**, 85, 1143-1154	2.9	36
248	Combined EXAFS, XRD, DRIFTS, and DFT Study of Nano Copper-Based Catalysts for CO2 Hydrogenation. *ACS Catalysis*, **2016**, 6, 5823-5833	13.1	35
247	Density-functional theory calculations of the interaction of protons and water with low-coordinated surface sites of calcium oxide. *Physical Review B*, **2001**, 63,	3.3	35
246	Enhancing the electrocatalytic activity of 2H-WS for hydrogen evolution via defect engineering. *Physical Chemistry Chemical Physics*, **2019**, 21, 6071-6079	3.6	35
245	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
244	A molecular dynamics study of the interprotein interactions in collagen fibrils. *Soft Matter*, **2011**, 7, 3373-3382	3.3	34
243	Hydrogen transfer and hydration properties of H(n)PO4(3-n) (n=0-3) in water studied by first principles molecular dynamics simulations. *Journal of Chemical Physics*, **2009**, 130, 234502	3.9	34
242	Deformation and Fracture of a SiO2 Nanorod. *Molecular Simulation*, **2003**, 29, 671-676	2	34
241	Surface structures, stabilities, and growth of magnesian calcites: A computational investigation from the perspective of dolomite formation. *American Mineralogist*, **2002**, 87, 679-689	2.9	34
240	The surface chemistry of NO(x) on mackinawite (FeS) surfaces: a DFT-D2 study. *Physical Chemistry Chemical Physics*, **2014**, 16, 15444-56	3.6	33
239	Ab initio molecular dynamics simulations of structural changes associated with the incorporation of fluorine in bioactive phosphate glasses. *Biomaterials*, **2014**, 35, 6164-71	15.6	33
238	Modelling the interaction of a Hyp-Pro-Gly peptide with hydroxyapatite surfaces in aqueous environment. *CrystEngComm*, **2010**, 12, 960-967	3.3	33

237	Phase separation and surface segregation in ceria–zirconia solid solutions. *Proceedings of the Royal Society A: Mathematical, Physical and Engineering Sciences*, **2011**, 467, 1925-1938	2.4	33
236	Distribution of Cations in FeSbO4: A Computer Modeling Study. *Chemistry of Materials*, **2004**, 16, 1954-1960	9.0	33
235	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
234	Density functional theory calculations of the hydrazine decomposition mechanism on the planar and stepped Cu(111) surfaces. *Physical Chemistry Chemical Physics*, **2015**, 17, 21533-46	3.6	31
233	The Role of Hydrogen Bonding and Proton Transfer in the Formation of Uracil Networks on the Gold (100) Surface: A Density Functional Theory Approach. *Journal of Physical Chemistry C*, **2013**, 117, 3949-3957	3.8	31
232	The surface structure of BaO on Pt(111): (2√7)-reconstructed BaO(111). *Surface Science*, **2006**, 600, 1973-1981	1.8	31
231	Calcium Phosphate Prenucleation Complexes in Water by Means of ab Initio Molecular Dynamics Simulations. *Crystal Growth and Design*, **2016**, 16, 3353-3358	3.5	30
230	Nanoscale chains control the solubility of phosphate glasses for biomedical applications. *Journal of Physical Chemistry B*, **2013**, 117, 10652-7	3.4	29
229	Mechanistic insights into the Cu(I) oxide-catalyzed conversion of CO2 to fuels and chemicals: A DFT approach. *Journal of CO2 Utilization*, **2016**, 15, 96-106	7.6	29
228	Polarizable force field development and molecular dynamics study of phosphate-based glasses. *Journal of Chemical Physics*, **2012**, 137, 234502	3.9	28
227	Thermochemistry of strontium incorporation in aragonite from atomistic simulations. *Geochimica Et Cosmochimica Acta*, **2010**, 74, 1320-1328	5.5	28
226	Advances in Sustainable Catalysis: A Computational Perspective. *Frontiers in Chemistry*, **2019**, 7, 182	5	27
225	A computer simulation study of the accommodation and diffusion of He in uranium- and plutonium-doped zircon (ZrSiO4). *Geochimica Et Cosmochimica Acta*, **2009**, 73, 3880-3893	5.5	27
224	Surface and shape modification of mackinawite (FeS) nanocrystals by cysteine adsorption: a first-principles DFT-D2 study. *Physical Chemistry Chemical Physics*, **2016**, 18, 32007-32020	3.6	27
223	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
222	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
221	Mixing thermodynamics of the calcite-structured (Mn,Ca)CO3 solid solution: a computer simulation study. *Journal of Physical Chemistry B*, **2011**, 115, 13854-61	3.4	26
220	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

219	Hydrogen adsorption on transition metal carbides: a DFT study. *Physical Chemistry Chemical Physics*, **2019**, 21, 5335-5343	3.6	25
218	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
217	Methanol formation from CO2 catalyzed by Fe3S4{111}: formate versus hydrocarboxyl pathways. *Faraday Discussions*, **2016**, 188, 161-80	3.6	25
216	Atomistic modeling of collagen proteins in their fibrillar environment. *Journal of Physical Chemistry B*, **2010**, 114, 13263-70	3.4	25
215	Interactions between Organophosphonate-Bearing Solutions and (101 4) Calcite Surfaces: An Atomic Force Microscopy and First-Principles Molecular Dynamics Study. *Crystal Growth and Design*, **2010**, 10, 3022-3035	3.5	25
214	Adsorption of methanoic acid onto the low-index surfaces of calcite and aragonite. *Molecular Simulation*, **2002**, 28, 539-556	2	25
213	Variations in calcite growth kinetics with surface topography: molecular dynamics simulations and process-based growth kinetics modelling. *CrystEngComm*, **2013**, 15, 5506	3.3	24
212	A computer modelling study of the interaction of organic adsorbates with fluorapatite surfaces. *Physics and Chemistry of Minerals*, **2006**, 33, 314-331	1.6	24
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210	Density functional theory study explaining the underperformance of copper oxides as photovoltaic absorbers. *Physical Review B*, **2019**, 99,	3.3	23
209	Where on Earth has our water come from?. *Chemical Communications*, **2010**, 46, 8923-5	5.8	23
208	Computer simulations of the effect of atomic structure and coordination on the stabilities and melting behaviour of copper surfaces and nano-particles. *Surface Science*, **2009**, 603, 445-454	1.8	23
207	Density-functional theory calculations of the adsorption of Cl at perfect and defective Ag(111) surfaces. *Physical Review B*, **2004**, 69,	3.3	23
206	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
205	A DFT+U investigation of hydrogen adsorption on the LaFeO(010) surface. *Physical Chemistry Chemical Physics*, **2017**, 19, 7399-7409	3.6	22
204	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
203	Ni Deposition on Yttria-Stabilized ZrO2(111) Surfaces: A Density Functional Theory Study. *Journal of Physical Chemistry C*, **2015**, 119, 6581-6591	3.8	22
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201	Thermodynamics of hydrogen vacancies in MgH2 from first-principles calculations and grand-canonical statistical mechanics. *Physical Review B*, **2009**, 80,	3.3	22
200	A Computer Modeling Study of Perfect and Defective Silver (111) Surfaces. *Journal of Physical Chemistry B*, **2003**, 107, 3528-3534	3.4	22
199	Properties of water confined in hydroxyapatite nanopores as derived from molecular dynamics simulations. *Theoretical Chemistry Accounts*, **2015**, 134, 1	1.9	21
198	Structural and Optical Properties of ZnO Thin Films Prepared by Molecular Precursor and Sol□el Methods. *Crystals*, **2020**, 10, 132	2.3	21
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	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
195	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
194	Periodic DFT+U investigation of the bulk and surface properties of marcasite (FeS). *Physical Chemistry Chemical Physics*, **2017**, 19, 27478-27488	3.6	21
193	A density functional theory investigation of the molecular and dissociative adsorption of hydrazine on defective copper surfaces. *Journal of Materials Chemistry*, **2012**, 22, 23210		21
192	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
191	Magnetic structure of UO and NpO by first-principle methods. *Physical Chemistry Chemical Physics*, **2019**, 21, 760-771	3.6	20
190	Hydrazine network on Cu(111) surface: A Density Functional Theory approach. *Surface Science*, **2015**, 637-638, 140-148	1.8	20
189	The effect of water on the binding of glycosaminoglycan saccharides to hydroxyapatite surfaces: a molecular dynamics study. *Physical Chemistry Chemical Physics*, **2015**, 17, 22377-88	3.6	20
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186	Density functional theory and interatomic potential study of structural, mechanical and surface properties of calcium oxalate materials. *RSC Advances*, **2012**, 2, 4664	3.7	20
185	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
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182	Transport properties of water molecules confined between hydroxyapaptite surfaces: A Molecular dynamics simulation approach. *Applied Surface Science*, **2017**, 418, 296-301	6.7	19
181	Modelling the structural evolution of ternary phosphate glasses from melts to solid amorphous materials. *Journal of Materials Chemistry B*, **2013**, 1, 5054-5066	7.3	19
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