Hendrik Heinz

List of Publications by Year
in descending order

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117 papers	9,333 citations	44069 48 h-index	39675 94 g-index
125 all docs	125 docs citations	125 times ranked	9047 citing authors

#	Article	IF	Citations
1	Accurate Simulation of Surfaces and Interfaces of Face-Centered Cubic Metals Using 12â^'6 and 9â^'6 Lennard-Jones Potentials. Journal of Physical Chemistry C, 2008, 112, 17281-17290.	3.1	792
2	Thermodynamically Consistent Force Fields for the Assembly of Inorganic, Organic, and Biological Nanostructures: The INTERFACE Force Field. Langmuir, 2013, 29, 1754-1765.	3.5	699
3	Nanoparticle decoration with surfactants: Molecular interactions, assembly, and applications. Surface Science Reports, 2017, 72, 1-58.	7.2	419
4	Force Field and a Surface Model Database for Silica to Simulate Interfacial Properties in Atomic Resolution. Chemistry of Materials, 2014, 26, 2647-2658.	6.7	369
5	Chemistry of Aqueous Silica Nanoparticle Surfaces and the Mechanism of Selective Peptide Adsorption. Journal of the American Chemical Society, 2012, 134, 6244-6256.	13.7	349
6	Nature of Molecular Interactions of Peptides with Gold, Palladium, and Pdâ^'Au Bimetal Surfaces in Aqueous Solution. Journal of the American Chemical Society, 2009, 131, 9704-9714.	13.7	334
7	Force Field for Mica-Type Silicates and Dynamics of Octadecylammonium Chains Grafted to Montmorillonite. Chemistry of Materials, 2005, 17, 5658-5669.	6.7	297
8	Self-Assembly of Alkylammonium Chains on Montmorillonite:Â Effect of Chain Length, Head Group Structure, and Cation Exchange Capacity. Chemistry of Materials, 2007, 19, 59-68.	6.7	248
9	Molecular models and simulations of layered materials. Journal of Materials Chemistry, 2009, 19, 2470.	6.7	244
10	Observing crystal nucleation in four dimensions using atomic electron tomography. Nature, 2019, 570, 500-503.	27.8	219
11	Atomic Charges for Classical Simulations of Polar Systems. Journal of Physical Chemistry B, 2004, 108, 18341-18352.	2.6	204
12	: A force field database for cementitious materials including validations, applications and opportunities. Cement and Concrete Research, 2017, 102, 68-89.	11.0	186
13	Adsorption mechanism of single amino acid and surfactant molecules to Au {111} surfaces in aqueous solution: design rules for metal-binding molecules. Soft Matter, 2011, 7, 2113.	2.7	185
14	Simulations of inorganicâ€"bioorganic interfaces to discover new materials: insights, comparisons to experiment, challenges, and opportunities. Chemical Society Reviews, 2016, 45, 412-448.	38.1	176
15	Three-dimensional coordinates of individual atoms in materials revealed by electronÂtomography. Nature Materials, 2015, 14, 1099-1103.	27.5	172
16	Structure and Phase Transitions of Alkyl Chains on Mica. Journal of the American Chemical Society, 2003, 125, 9500-9510.	13.7	164
17	Building two-dimensional materials one row at a time: Avoiding the nucleation barrier. Science, 2018, 362, 1135-1139.	12.6	155
18	Influence of aluminates on the hydration kinetics of tricalcium silicate. Cement and Concrete Research, 2017, 100, 245-262.	11.0	146

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19	Carbon Nanotube Dispersion in Solvents and Polymer Solutions: Mechanisms, Assembly, and Preferences. ACS Nano, 2017, 11, 12805-12816.	14.6	145
20	Force Field for Tricalcium Silicate and Insight into Nanoscale Properties: Cleavage, Initial Hydration, and Adsorption of Organic Molecules. Journal of Physical Chemistry C, 2013, 117, 10417-10432.	3.1	141
21	Accurate Force Field Parameters and pH Resolved Surface Models for Hydroxyapatite to Understand Structure, Mechanics, Hydration, and Biological Interfaces. Journal of Physical Chemistry C, 2016, 120, 4975-4992.	3.1	139
22	Prediction of Specific Biomolecule Adsorption on Silica Surfaces as a Function of pH and Particle Size. Chemistry of Materials, 2014, 26, 5725-5734.	6.7	125
23	Insight into induced charges at metal surfaces and biointerfaces using a polarizable Lennardâ€“Jones potential. Nature Communications, 2018, 9, 716.	12.8	121
24	Interaction energy and surface reconstruction between sheets of layered silicates. Journal of Chemical Physics, 2006, 124, 224713.	3.0	113
25	Tailoring Molecular Specificity Toward a Crystal Facet: a Lesson From Biorecognition Toward Pt{111}. Nano Letters, 2013, 13, 840-846.	9.1	101
26	Crystallographic Recognition Controls Peptide Binding for Bio-Based Nanomaterials. Journal of the American Chemical Society, 2011, 133, 12346-12349.	13.7	96
27	Elucidation of Peptide-Directed Palladium Surface Structure for Biologically Tunable Nanocatalysts. ACS Nano, 2015, 9, 5082-5092.	14.6	96
28	Cleavage Energy of Alkylammonium-Modified Montmorillonite and Relation to Exfoliation in Nanocomposites: Influence of Cation Density, Head Group Structure, and Chain Length. Chemistry of Materials, 2010, 22, 1595-1605.	6.7	95
29	Relation between Packing Density and Thermal Transitions of Alkyl Chains on Layered Silicate and Metal Surfaces. Langmuir, 2008, 24, 3727-3733.	3.5	94
30	Single- and multi-component chiral supraparticles as modular enantioselective catalysts. Nature Communications, 2019, 10, 4826.	12.8	93
31	Influence of the Shape of Nanostructured Metal Surfaces on Adsorption of Single Peptide Molecules in Aqueous Solution. Small, 2012, 8, 1049-1059.	10.0	92
32	Adsorption of peptides (A3, Flg, Pd2, Pd4) on gold and palladium surfaces by a coarse-grained Monte Carlo simulation. Physical Chemistry Chemical Physics, 2009, 11, 1989.	2.8	87
33	A force field for tricalcium aluminate to characterize surface properties, initial hydration, and organically modified interfaces in atomic resolution. Dalton Transactions, 2014, 43, 10602-10616.	3.3	87
34	Exploiting Localized Surface Binding Effects to Enhance the Catalytic Reactivity of Peptide-Capped Nanoparticles. Journal of the American Chemical Society, 2013, 135, 11048-11054.	13.7	86
35	Toward Understanding Amino Acid Adsorption at Metallic Interfaces: A Density Functional Theory Study. ACS Applied Materials & Interfaces, 2009, 1, 388-392.	8.0	85
36	Photoisomerization of Azobenzene Grafted to Layered Silicates: Simulation and Experimental Challenges. Chemistry of Materials, 2008, 20, 6444-6456.	6.7	82

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37	Clay minerals for nanocomposites and biotechnology: surface modification, dynamics and responses to stimuli. Clay Minerals, 2012, 47, 205-230.	0.6	81
38	Facet Recognition and Molecular Ordering of Ionic Liquids on Metal Surfaces. Journal of Physical Chemistry C, 2013, 117, 25969-25981.	3.1	80
39	Surface Structure of Organoclays. Angewandte Chemie - International Edition, 2004, 43, 2239-2243.	13.8	76
40	Calculation of local pressure tensors in systems with many-body interactions. Physical Review E, 2005, 72, 066704.	2.1	66
41	Polarization at metalâ€“biomolecular interfaces in solution. Journal of the Royal Society Interface, 2011, 8, 220-232.	3.4	66
42	Molecular Mechanism of Specific Recognition of Cubic Pt Nanocrystals by Peptides and of the Concentrationâ€Đependent Formation from Seed Crystals. Advanced Functional Materials, 2015, 25, 1374-1384.	14.9	65
43	Nanoscale Tensile, Shear, and Failure Properties of Layered Silicates as a Function of Cation Density and Stress. Journal of Physical Chemistry C, 2010, 114, 1763-1772.	3.1	64
44	Molecular engineering of interphases in polymer/carbon nanotube composites to reach the limits of mechanical performance. Composites Science and Technology, 2018, 166, 86-94.	7.8	59
45	Bending of Layered Silicates on the Nanometer Scale: Mechanism, Stored Energy, and Curvature Limits. Journal of Physical Chemistry C, 2011, 115, 22292-22300.	3.1	57
46	Stability, surface features, and atom leaching of palladium nanoparticles: toward prediction of catalytic functionality. Physical Chemistry Chemical Physics, 2013, 15, 5488.	2.8	57
47	Computational screening of biomolecular adsorption and selfâ€assembly on nanoscale surfaces. Journal of Computational Chemistry, 2010, 31, 1564-1568.	3.3	56
48	Dynamics of Alkyl Ammonium Intercalants within Organically Modified Montmorillonite:Â Dielectric Relaxation and Ionic Conductivity. Journal of Physical Chemistry B, 2006, 110, 20143-20157.	2.6	53
49	CHARMM-GUI Nanomaterial Modeler for Modeling and Simulation of Nanomaterial Systems. Journal of Chemical Theory and Computation, 2022, 18, 479-493.	5.3	53
50	A Rational Biomimetic Approach to Structure Defect Generation in Colloidal Nanocrystals. ACS Nano, 2014, 8, 6934-6944.	14.6	49
51	Atomic-scale identification of Pd leaching in nanoparticle catalyzed Câ€“C coupling: effects of particle surface disorder. Chemical Science, 2015, 6, 6413-6419.	7.4	44
52	Peptide-Assisted 2-D Assembly toward Free-Floating Ultrathin Platinum Nanoplates as Effective Electrocatalysts. Nano Letters, 2019, 19, 3730-3736.	9.1	44
53	Involvement of prenucleation clusters in calcium phosphate mineralization of collagen. Acta Biomaterialia, 2021, 120, 213-223.	8.3	44
54	Direct correlation of oxygen adsorption on platinum-electrolyte interfaces with the activity in the oxygen reduction reaction. Science Advances, 2021, 7, .	10.3	44

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55	Nanoscale Structureâ€“Property Relationships of Polyacrylonitrile/CNT Composites as a Function of Polymer Crystallinity and CNT Diameter. ACS Applied Materials & Interfaces, 2018, 10, 1017-1027.	8.0	43
56	Atomic-Scale Structure and Stress Release Mechanism in Coreâ€“Shell Nanoparticles. ACS Nano, 2018, 12, 12296-12304.	14.6	41
57	Mechanism of molecular interaction of acrylate-polyethylene glycol acrylate copolymers with calcium silicate hydrate surfaces. Green Chemistry, 2020, 22, 1577-1593.	9.0	38
58	Molecular Dynamics Modeling of Epoxy Resins Using the Reactive Interface Force Field. Macromolecules, 2021, 54, 9815-9824.	4.8	37
59	Accurate and Compatible Force Fields for Molecular Oxygen, Nitrogen, and Hydrogen to Simulate Gases, Electrolytes, and Heterogeneous Interfaces. Journal of Chemical Theory and Computation, 2021, 17, 5198-5213.	5.3	36
60	Force field for calcium sulfate minerals to predict structural, hydration, and interfacial properties. Cement and Concrete Research, 2021, 139, 106262.	11.0	35
61	Reliable computational design of biological-inorganic materials to the large nanometer scale using Interface-FF. Molecular Simulation, 2017, 43, 1394-1405.	2.0	34
62	Interpretable molecular models for molybdenum disulfide and insight into selective peptide recognition. Chemical Science, 2020, 11, 8708-8722.	7.4	32
63	Understanding the Surface Reactivity of Ligand-Protected Metal Nanoparticles for Biomass Upgrading. ACS Catalysis, 2020, 10, 5462-5474.	11.2	32
64	ReaxFF Reactive Force Field Study of Polymerization of a Polymer Matrix in a Carbon Nanotube-Composite System. Journal of Physical Chemistry C, 2020, 124, 20488-20497.	3.1	31
65	Analysis of the phase transitions in alkyl-mica by density and pressure profiles. Journal of Chemical Physics, 2004, 120, 3847-3854.	3.0	30
66	Understanding Chemical Bonding in Alloys and the Representation in Atomistic Simulations. Journal of Physical Chemistry C, 2018, 122, 14996-15009.	3.1	30
67	Nature of peptide wrapping onto metal nanoparticle catalysts and driving forces for size control. Nanoscale, 2017, 9, 8401-8409.	5.6	29
68	Accurate simulation of surfaces and interfaces of ten FCC metals and steel using Lennardâ€“Jones potentials. Npj Computational Materials, 2021, 7, .	8.7	28
69	Adsorption of biomolecules and polymers on silicates, glasses, and oxides: mechanisms, predictions, and opportunities by molecular simulation. Current Opinion in Chemical Engineering, 2016, 11, 34-41.	7.8	26
70	Conformation and dynamics of a self-avoiding sheet: Bond-fluctuation computer simulation. Journal of Polymer Science, Part B: Polymer Physics, 2005, 43, 1041-1046.	2.1	23
71	Calculation of local and average pressure tensors in molecular simulations. Molecular Simulation, 2007, 33, 747-758.	2.0	23
72	Structure and cleavage energy of surfactant-modified clay minerals: Influence of CEC, head group and chain length. Philosophical Magazine, 2010, 90, 2415-2424.	1.6	23

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73	Adsorption and Substitution of Metal Ions on Hydroxyapatite as a Function of Crystal Facet and Electrolyte pH. Journal of Physical Chemistry C, 2019, 123, 16982-16993.	3.1	22
74	Working Mechanisms and Design Principles of Comb-like Polycarboxylate Ether Superplasticizers in Cement Hydration: Quantitative Insights for a Series of Well-Defined Copolymers. ACS Sustainable Chemistry and Engineering, 2021, 9, 8354-8371.	6.7	22
75	Simple and Accurate Computations of Solvatochromic Shifts in Ï€ â†' Ï€* Transitions of Aromatic Chromophores. Journal of the American Chemical Society, 2001, 123, 11229-11236.	13.7	21
76	Long-Range Hierarchical Nanocrystal Assembly Driven by Molecular Structural Transformation. Journal of the American Chemical Society, 2019, 141, 1498-1505.	13.7	21
77	Energy-effective Grinding of Inorganic Solids Using Organic Additives. Chimia, 2017, 71, 451.	0.6	19
78	Polyacrylonitrile Interactions with Carbon Nanotubes in Solution: Conformations and Binding as a Function of Solvent, Temperature, and Concentration. Advanced Functional Materials, 2019, 29, 1905247.	14.9	19
79	Amyloid-like amelogenin nanoribbons template mineralization via a low-energy interface of ion binding sites. Proceedings of the National Academy of Sciences of the United States of America, 2022, 119, e2106965119.	7.1	19
80	Control over Self-Assembly of Diblock Copolymers on Hexagonal and Square Templates for High Area Density Circuit Boards. ACS Nano, 2011, 5, 9413-9420.	14.6	18
81	Interactions at the Silicaâ€“Peptide Interface: Influence of the Extent of Functionalization on the Conformational Ensemble. Langmuir, 2018, 34, 8255-8263.	3.5	18
82	The role of chemistry and pH of solid surfaces for specific adsorption of biomolecules in solutionâ€"accurate computational models and experiment. Journal of Physics Condensed Matter, 2014, 26, 244105.	1.8	17
83	Enhancement of oxygen reduction reaction activity by grain boundaries in platinum nanostructures. Nano Research, 2020, 13, 3310-3314.	10.4	17
84	Vaporizable endoskeletal droplets via tunable interfacial melting transitions. Science Advances, 2020, 6, eaaz7188.	10.3	16
85	Cement Interfaces: Current Understanding, Challenges, and Opportunities. Langmuir, 2021, 37, 6347-6356.	3.5	16
86	Binding mechanism and binding free energy of amino acids and citrate to hydroxyapatite surfaces as a function of crystallographic facet, pH, and electrolytes. Journal of Colloid and Interface Science, 2022, 605, 685-700.	9.4	16
87	Molecular modeling of chemical admixtures; opportunities and challenges. Cement and Concrete Research, 2022, 156, 106783.	11.0	16
88	Normal and defective perylene substitution sites in alkane crystals. Journal of Chemical Physics, 2001, 114, 3224-3235.	3.0	15
89	Investigation of nanostructures and properties of sulfonated poly(arylenethioethersulfone) copolymer as proton conducting materials by small angle neutron scattering. Polymer, 2010, 51, 1585-1592.	3.8	14
90	Morphology of sulfonated polyarylenethioethersulfone random copolymer series as proton exchange fuel cells membranes by small angle neutron scattering. Polymer, 2011, 52, 5615-5621.	3.8	14

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91	Interaction of substituted poly(phenyleneethynylene)s with ligand-stabilized CdS nanoparticles. Journal of Materials Chemistry A, 2014, 2, 8705-8711.	10.3	13
92	Dynamics of carbohydrate strands in water and interactions with clay minerals: influence of pH, surface chemistry, and electrolytes. Nanoscale, 2019, 11, 11183-11194.	5.6	13
93	Molecular dynamics simulations of separator-cathode interfacial thermal transport in a Li-ion cell. Surfaces and Interfaces, 2020, 21, 100674.	3.0	11
94	Patterning of Self-Assembled Monolayers of Amphiphilic Multisegment Ligands on Nanoparticles and Design Parameters for Protein Interactions. ACS Nano, 2022, 16, 8766-8783.	14.6	11
95	Furfuryl alcohol deoxygenation, decarbonylation, and ring-opening on Pt(111). Surface Science, 2018, 677, 333-340.	1.9	10
96	Single-shot 3D coherent diffractive imaging of core-shell nanoparticles with elemental specificity. Scientific Reports, 2018, 8, 8284.	3.3	10
97	From phage display to structure: an interplay of enthalpy and entropy in the binding of the LDHSLHS polypeptide to silica. Physical Chemistry Chemical Physics, 2019, 21, 4663-4672.	2.8	9
98	Layer of clay platelets in a peptide matrix: Binding, encapsulation, and morphology. Journal of Polymer Science, Part B: Polymer Physics, 2010, 48, 2566-2574.	2.1	7
99	Molecular structure and assembly of peptide-derived nanomaterials. Current Opinion in Green and Sustainable Chemistry, 2018, 12, 38-46.	5.9	6
100	Quantitative characterization of high temperature oxidation using electron tomography and energy-dispersive X-ray spectroscopy. Scientific Reports, 2018, 8, 10239.	3.3	6
101	Reactive modeling of Mo3Si oxidation and resulting silica morphology. Acta Materialia, 2020, 187, 93-102.	7.9	6
102	Biofunctionalization and immobilization of a membrane via peptide binding (CR3-1, S2) by a Monte Carlo simulation. Journal of Chemical Physics, 2010, 133, 095102.	3.0	5
103	Constructing surface models of silicate glasses using molecular dynamics to understand the effect of pH on the hydration properties. Journal of Chemical Physics, 2019, 150, 174703.	3.0	5
104	Post-synthetic modification of ionic liquids using ligand-exchange and redox coordination chemistry. Journal of Materials Chemistry A, 2020, 8, 22674-22685.	10.3	5
105	Interaction of Poly(methyl acrylate) with Carbon Nanotubes as a Function of CNT Diameter, Chirality, and Temperature. Journal of Physical Chemistry C, 2020, 124, 25632-25644.	3.1	4
106	Adsorption and Diffusion of Oxygen on Pure and Partially Oxidized Metal Surfaces in Ultrahigh Resolution. Nano Letters, 2022, 22, 5392-5400.	9.1	4
107	UV-Absorption and Silica/Titania Colloids Using a Coreâ€“Shell Approach. Silicon, 2010, 2, 95-104.	3.3	3
108	Study of the Impact of Polyanions on the Formation of Lipid Bilayers on Top of Polyelectrolyte Multilayers with Poly(allylamine hydrochloride) as the Top Layer. Journal of Physical Chemistry B, 2017, 121, 1158-1167.	2.6	2

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109	Binding of polar and hydrophobic molecules at the LiCoO₂ (001)-water interface: force field development and molecular dynamics simulations. Nanoscale, 2022, , .	5.6	2
110	Multiscale Experiments and Modeling in Biomaterials and Biological Materials, Part I. Jom, 2021, 73, 1673-1675.	1.9	1
111	Surface patterning in alloys. , 2022, 1, 103-104.		1
112	Three-Dimensional Determination of the Coordinates of Individual Atoms in Materials. Microscopy and Microanalysis, 2016, 22, 916-917.	0.4	0
113	4D Atomic Electron Tomography. Microscopy and Microanalysis, 2019, 25, 1814-1815.	0.4	0
114	Imaging Nucleation, Growth and Disorder at the Single-atom Level by Atomic Electron Tomography (AET). Microscopy and Microanalysis, 2020, 26, 1848-1850.	0.4	0
115	Multiscale Experiments and Modeling in Biomaterials and Biological Materials, Part II. Jom, 2021, 73, 2332-2334.	1.9	0
116	Anchoring of a hydrophobic heptapeptide (AFILPTG) on silica facilitates peptide unfolding at the abioticâ€“biotic interface. Physical Chemistry Chemical Physics, 2021, 23, 18001-18011.	2.8	0
117	Understanding Molecular Recognition on Metallic and Oxidic Nanostructures from a Perspective of Computer Simulation and Theory. , 2014, , 141-171.		0