

# 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	Binding mechanism and binding free energy of amino acids and citrate to hydroxyapatite surfaces as a function of crystallographic facet, pH, and electrolytes. <i>Journal of Colloid and Interface Science</i> , 2022, 605, 685-700.	9.4	16
2	Surface patterning in alloys. , 2022, 1, 103-104.		1
3	Molecular modeling of chemical admixtures; opportunities and challenges. <i>Cement and Concrete Research</i> , 2022, 156, 106783.	11.0	16
4	CHARMM-GUI Nanomaterial Modeler for Modeling and Simulation of Nanomaterial Systems. <i>Journal of Chemical Theory and Computation</i> , 2022, 18, 479-493.	5.3	53
5	Binding of polar and hydrophobic molecules at the LiCoO <sub>2</sub> (001)-water interface: force field development and molecular dynamics simulations. <i>Nanoscale</i> , 2022, , .	5.6	2
6	Amyloid-like amelogenin nanoribbons template mineralization via a low-energy interface of ion binding sites. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2022, 119, e2106965119.	7.1	19
7	Patterning of Self-Assembled Monolayers of Amphiphilic Multisegment Ligands on Nanoparticles and Design Parameters for Protein Interactions. <i>ACS Nano</i> , 2022, 16, 8766-8783.	14.6	11
8	Adsorption and Diffusion of Oxygen on Pure and Partially Oxidized Metal Surfaces in Ultrahigh Resolution. <i>Nano Letters</i> , 2022, 22, 5392-5400.	9.1	4
9	Involvement of prenucleation clusters in calcium phosphate mineralization of collagen. <i>Acta Biomaterialia</i> , 2021, 120, 213-223.	8.3	44
10	Force field for calcium sulfate minerals to predict structural, hydration, and interfacial properties. <i>Cement and Concrete Research</i> , 2021, 139, 106262.	11.0	35
11	Multiscale Experiments and Modeling in Biomaterials and Biological Materials, Part I. <i>Jom</i> , 2021, 73, 1673-1675.	1.9	1
12	Cement Interfaces: Current Understanding, Challenges, and Opportunities. <i>Langmuir</i> , 2021, 37, 6347-6356.	3.5	16
13	Working Mechanisms and Design Principles of Comb-like Polycarboxylate Ether Superplasticizers in Cement Hydration: Quantitative Insights for a Series of Well-Defined Copolymers. <i>ACS Sustainable Chemistry and Engineering</i> , 2021, 9, 8354-8371.	6.7	22
14	Direct correlation of oxygen adsorption on platinum-electrolyte interfaces with the activity in the oxygen reduction reaction. <i>Science Advances</i> , 2021, 7, .	10.3	44
15	Multiscale Experiments and Modeling in Biomaterials and Biological Materials, Part II. <i>Jom</i> , 2021, 73, 2332-2334.	1.9	0
16	Accurate and Compatible Force Fields for Molecular Oxygen, Nitrogen, and Hydrogen to Simulate Gases, Electrolytes, and Heterogeneous Interfaces. <i>Journal of Chemical Theory and Computation</i> , 2021, 17, 5198-5213.	5.3	36
17	Anchoring of a hydrophobic heptapeptide (AFILPTG) on silica facilitates peptide unfolding at the abiotic–biotic interface. <i>Physical Chemistry Chemical Physics</i> , 2021, 23, 18001-18011.	2.8	0
18	Accurate simulation of surfaces and interfaces of ten FCC metals and steel using Lennard–Jones potentials. <i>Npj Computational Materials</i> , 2021, 7, .	8.7	28

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19	Molecular Dynamics Modeling of Epoxy Resins Using the Reactive Interface Force Field. <i>Macromolecules</i> , 2021, 54, 9815-9824.	4.8	37
20	Mechanism of molecular interaction of acrylate-polyethylene glycol acrylate copolymers with calcium silicate hydrate surfaces. <i>Green Chemistry</i> , 2020, 22, 1577-1593.	9.0	38
21	Post-synthetic modification of ionic liquids using ligand-exchange and redox coordination chemistry. <i>Journal of Materials Chemistry A</i> , 2020, 8, 22674-22685.	10.3	5
22	Imaging Nucleation, Growth and Disorder at the Single-atom Level by Atomic Electron Tomography (AET). <i>Microscopy and Microanalysis</i> , 2020, 26, 1848-1850.	0.4	0
23	Interpretable molecular models for molybdenum disulfide and insight into selective peptide recognition. <i>Chemical Science</i> , 2020, 11, 8708-8722.	7.4	32
24	Enhancement of oxygen reduction reaction activity by grain boundaries in platinum nanostructures. <i>Nano Research</i> , 2020, 13, 3310-3314.	10.4	17
25	Molecular dynamics simulations of separator-cathode interfacial thermal transport in a Li-ion cell. <i>Surfaces and Interfaces</i> , 2020, 21, 100674.	3.0	11
26	ReaxFF Reactive Force Field Study of Polymerization of a Polymer Matrix in a Carbon Nanotube-Composite System. <i>Journal of Physical Chemistry C</i> , 2020, 124, 20488-20497.	3.1	31
27	Interaction of Poly(methyl acrylate) with Carbon Nanotubes as a Function of CNT Diameter, Chirality, and Temperature. <i>Journal of Physical Chemistry C</i> , 2020, 124, 25632-25644.	3.1	4
28	Reactive modeling of Mo <sub>3</sub> Si oxidation and resulting silica morphology. <i>Acta Materialia</i> , 2020, 187, 93-102.	7.9	6
29	Understanding the Surface Reactivity of Ligand-Protected Metal Nanoparticles for Biomass Upgrading. <i>ACS Catalysis</i> , 2020, 10, 5462-5474.	11.2	32
30	Vaporizable endoskeletal droplets via tunable interfacial melting transitions. <i>Science Advances</i> , 2020, 6, eaaz7188.	10.3	16
31	Polyacrylonitrile Interactions with Carbon Nanotubes in Solution: Conformations and Binding as a Function of Solvent, Temperature, and Concentration. <i>Advanced Functional Materials</i> , 2019, 29, 1905247.	14.9	19
32	Single- and multi-component chiral supraparticles as modular enantioselective catalysts. <i>Nature Communications</i> , 2019, 10, 4826.	12.8	93
33	4D Atomic Electron Tomography. <i>Microscopy and Microanalysis</i> , 2019, 25, 1814-1815.	0.4	0
34	From phage display to structure: an interplay of enthalpy and entropy in the binding of the LDHSLHS polypeptide to silica. <i>Physical Chemistry Chemical Physics</i> , 2019, 21, 4663-4672.	2.8	9
35	Dynamics of carbohydrate strands in water and interactions with clay minerals: influence of pH, surface chemistry, and electrolytes. <i>Nanoscale</i> , 2019, 11, 11183-11194.	5.6	13
36	Observing crystal nucleation in four dimensions using atomic electron tomography. <i>Nature</i> , 2019, 570, 500-503.	27.8	219

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37	Constructing surface models of silicate glasses using molecular dynamics to understand the effect of pH on the hydration properties. <i>Journal of Chemical Physics</i> , 2019, 150, 174703.	3.0	5
38	Peptide-Assisted 2-D Assembly toward Free-Floating Ultrathin Platinum Nanoplates as Effective Electrocatalysts. <i>Nano Letters</i> , 2019, 19, 3730-3736.	9.1	44
39	Adsorption and Substitution of Metal Ions on Hydroxyapatite as a Function of Crystal Facet and Electrolyte pH. <i>Journal of Physical Chemistry C</i> , 2019, 123, 16982-16993.	3.1	22
40	Long-Range Hierarchical Nanocrystal Assembly Driven by Molecular Structural Transformation. <i>Journal of the American Chemical Society</i> , 2019, 141, 1498-1505.	13.7	21
41	Molecular engineering of interphases in polymer/carbon nanotube composites to reach the limits of mechanical performance. <i>Composites Science and Technology</i> , 2018, 166, 86-94.	7.8	59
42	Insight into induced charges at metal surfaces and biointerfaces using a polarizable Lennard-Jones potential. <i>Nature Communications</i> , 2018, 9, 716.	12.8	121
43	Nanoscale Structure-Property Relationships of Polyacrylonitrile/CNT Composites as a Function of Polymer Crystallinity and CNT Diameter. <i>ACS Applied Materials &amp; Interfaces</i> , 2018, 10, 1017-1027.	8.0	43
44	Atomic-Scale Structure and Stress Release Mechanism in Core-Shell Nanoparticles. <i>ACS Nano</i> , 2018, 12, 12296-12304.	14.6	41
45	Building two-dimensional materials one row at a time: Avoiding the nucleation barrier. <i>Science</i> , 2018, 362, 1135-1139.	12.6	155
46	Furfuryl alcohol deoxygenation, decarbonylation, and ring-opening on Pt(111). <i>Surface Science</i> , 2018, 677, 333-340.	1.9	10
47	Single-shot 3D coherent diffractive imaging of core-shell nanoparticles with elemental specificity. <i>Scientific Reports</i> , 2018, 8, 8284.	3.3	10
48	Understanding Chemical Bonding in Alloys and the Representation in Atomistic Simulations. <i>Journal of Physical Chemistry C</i> , 2018, 122, 14996-15009.	3.1	30
49	Molecular structure and assembly of peptide-derived nanomaterials. <i>Current Opinion in Green and Sustainable Chemistry</i> , 2018, 12, 38-46.	5.9	6
50	Interactions at the Silica-Peptide Interface: Influence of the Extent of Functionalization on the Conformational Ensemble. <i>Langmuir</i> , 2018, 34, 8255-8263.	3.5	18
51	Quantitative characterization of high temperature oxidation using electron tomography and energy-dispersive X-ray spectroscopy. <i>Scientific Reports</i> , 2018, 8, 10239.	3.3	6
52	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. <i>Journal of Physical Chemistry B</i> , 2017, 121, 1158-1167.	2.6	2
53	Nanoparticle decoration with surfactants: Molecular interactions, assembly, and applications. <i>Surface Science Reports</i> , 2017, 72, 1-58.	7.2	419
54	Reliable computational design of biological-inorganic materials to the large nanometer scale using Interface-FF. <i>Molecular Simulation</i> , 2017, 43, 1394-1405.	2.0	34

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55	: A force field database for cementitious materials including validations, applications and opportunities. Cement and Concrete Research, 2017, 102, 68-89.	11.0	186
56	Influence of aluminates on the hydration kinetics of tricalcium silicate. Cement and Concrete Research, 2017, 100, 245-262.	11.0	146
57	Nature of peptide wrapping onto metal nanoparticle catalysts and driving forces for size control. Nanoscale, 2017, 9, 8401-8409.	5.6	29
58	Carbon Nanotube Dispersion in Solvents and Polymer Solutions: Mechanisms, Assembly, and Preferences. ACS Nano, 2017, 11, 12805-12816.	14.6	145
59	Energy-effective Grinding of Inorganic Solids Using Organic Additives. Chimia, 2017, 71, 451.	0.6	19
60	Three-Dimensional Determination of the Coordinates of Individual Atoms in Materials. Microscopy and Microanalysis, 2016, 22, 916-917.	0.4	0
61	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
62	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
63	Simulations of inorganic-bioorganic interfaces to discover new materials: insights, comparisons to experiment, challenges, and opportunities. Chemical Society Reviews, 2016, 45, 412-448.	38.1	176
64	Molecular Mechanism of Specific Recognition of Cubic Pt Nanocrystals by Peptides and of the Concentration-Dependent Formation from Seed Crystals. Advanced Functional Materials, 2015, 25, 1374-1384.	14.9	65
65	Atomic-scale identification of Pd leaching in nanoparticle catalyzed C-C coupling: effects of particle surface disorder. Chemical Science, 2015, 6, 6413-6419.	7.4	44
66	Elucidation of Peptide-Directed Palladium Surface Structure for Biologically Tunable Nanocatalysts. ACS Nano, 2015, 9, 5082-5092.	14.6	96
67	Three-dimensional coordinates of individual atoms in materials revealed by electron tomography. Nature Materials, 2015, 14, 1099-1103.	27.5	172
68	Interaction of substituted poly(phenyleneethynylene)s with ligand-stabilized CdS nanoparticles. Journal of Materials Chemistry A, 2014, 2, 8705-8711.	10.3	13
69	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
70	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
71	The role of chemistry and pH of solid surfaces for specific adsorption of biomolecules in solution: accurate computational models and experiment. Journal of Physics Condensed Matter, 2014, 26, 244105.	1.8	17
72	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

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73	A Rational Biomimetic Approach to Structure Defect Generation in Colloidal Nanocrystals. ACS Nano, 2014, 8, 6934-6944.	14.6	49
74	Understanding Molecular Recognition on Metallic and Oxidic Nanostructures from a Perspective of Computer Simulation and Theory. , 2014, , 141-171.		0
75	Stability, surface features, and atom leaching of palladium nanoparticles: toward prediction of catalytic functionality. Physical Chemistry Chemical Physics, 2013, 15, 5488.	2.8	57
76	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
77	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
78	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
79	Facet Recognition and Molecular Ordering of Ionic Liquids on Metal Surfaces. Journal of Physical Chemistry C, 2013, 117, 25969-25981.	3.1	80
80	Tailoring Molecular Specificity Toward a Crystal Facet: a Lesson From Biorecognition Toward Pt{111}. Nano Letters, 2013, 13, 840-846.	9.1	101
81	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
82	Clay minerals for nanocomposites and biotechnology: surface modification, dynamics and responses to stimuli. Clay Minerals, 2012, 47, 205-230.	0.6	81
83	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
84	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
85	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
86	Crystallographic Recognition Controls Peptide Binding for Bio-Based Nanomaterials. Journal of the American Chemical Society, 2011, 133, 12346-12349.	13.7	96
87	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
88	Polarization at metal-biomolecular interfaces in solution. Journal of the Royal Society Interface, 2011, 8, 220-232.	3.4	66
89	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
90	Computational screening of biomolecular adsorption and self-assembly on nanoscale surfaces. Journal of Computational Chemistry, 2010, 31, 1564-1568.	3.3	56

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91	UV-Absorption and Silica/Titania Colloids Using a Core-Shell Approach. <i>Silicon</i> , 2010, 2, 95-104.	3.3	3
92	Investigation of nanostructures and properties of sulfonated poly(arylenethioethersulfone) copolymer as proton conducting materials by small angle neutron scattering. <i>Polymer</i> , 2010, 51, 1585-1592.	3.8	14
93	Layer of clay platelets in a peptide matrix: Binding, encapsulation, and morphology. <i>Journal of Polymer Science, Part B: Polymer Physics</i> , 2010, 48, 2566-2574.	2.1	7
94	Biofunctionalization and immobilization of a membrane via peptide binding (CR3-1, S2) by a Monte Carlo simulation. <i>Journal of Chemical Physics</i> , 2010, 133, 095102.	3.0	5
95	Cleavage Energy of Alkylammonium-Modified Montmorillonite and Relation to Exfoliation in Nanocomposites: Influence of Cation Density, Head Group Structure, and Chain Length. <i>Chemistry of Materials</i> , 2010, 22, 1595-1605.	6.7	95
96	Nanoscale Tensile, Shear, and Failure Properties of Layered Silicates as a Function of Cation Density and Stress. <i>Journal of Physical Chemistry C</i> , 2010, 114, 1763-1772.	3.1	64
97	Structure and cleavage energy of surfactant-modified clay minerals: Influence of CEC, head group and chain length. <i>Philosophical Magazine</i> , 2010, 90, 2415-2424.	1.6	23
98	Toward Understanding Amino Acid Adsorption at Metallic Interfaces: A Density Functional Theory Study. <i>ACS Applied Materials &amp; Interfaces</i> , 2009, 1, 388-392.	8.0	85
99	Molecular models and simulations of layered materials. <i>Journal of Materials Chemistry</i> , 2009, 19, 2470.	6.7	244
100	Nature of Molecular Interactions of Peptides with Gold, Palladium, and Pd-Au Bimetal Surfaces in Aqueous Solution. <i>Journal of the American Chemical Society</i> , 2009, 131, 9704-9714.	13.7	334
101	Adsorption of peptides (A3, Flg, Pd2, Pd4) on gold and palladium surfaces by a coarse-grained Monte Carlo simulation. <i>Physical Chemistry Chemical Physics</i> , 2009, 11, 1989.	2.8	87
102	Accurate Simulation of Surfaces and Interfaces of Face-Centered Cubic Metals Using $12\text{-}\sigma^6$ and $9\text{-}\sigma^6$ Lennard-Jones Potentials. <i>Journal of Physical Chemistry C</i> , 2008, 112, 17281-17290.	3.1	792
103	Photoisomerization of Azobenzene Grafted to Layered Silicates: Simulation and Experimental Challenges. <i>Chemistry of Materials</i> , 2008, 20, 6444-6456.	6.7	82
104	Relation between Packing Density and Thermal Transitions of Alkyl Chains on Layered Silicate and Metal Surfaces. <i>Langmuir</i> , 2008, 24, 3727-3733.	3.5	94
105	Calculation of local and average pressure tensors in molecular simulations. <i>Molecular Simulation</i> , 2007, 33, 747-758.	2.0	23
106	Self-Assembly of Alkylammonium Chains on Montmorillonite: Effect of Chain Length, Head Group Structure, and Cation Exchange Capacity. <i>Chemistry of Materials</i> , 2007, 19, 59-68.	6.7	248
107	Interaction energy and surface reconstruction between sheets of layered silicates. <i>Journal of Chemical Physics</i> , 2006, 124, 224713.	3.0	113
108	Dynamics of Alkyl Ammonium Intercalants within Organically Modified Montmorillonite: Dielectric Relaxation and Ionic Conductivity. <i>Journal of Physical Chemistry B</i> , 2006, 110, 20143-20157.	2.6	53

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109	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
110	Force Field for Mica-Type Silicates and Dynamics of Octadecylammonium Chains Grafted to Montmorillonite. Chemistry of Materials, 2005, 17, 5658-5669.	6.7	297
111	Calculation of local pressure tensors in systems with many-body interactions. Physical Review E, 2005, 72, 066704.	2.1	66
112	Surface Structure of Organoclays. Angewandte Chemie - International Edition, 2004, 43, 2239-2243.	13.8	76
113	Analysis of the phase transitions in alkyl-mica by density and pressure profiles. Journal of Chemical Physics, 2004, 120, 3847-3854.	3.0	30
114	Atomic Charges for Classical Simulations of Polar Systems. Journal of Physical Chemistry B, 2004, 108, 18341-18352.	2.6	204
115	Structure and Phase Transitions of Alkyl Chains on Mica. Journal of the American Chemical Society, 2003, 125, 9500-9510.	13.7	164
116	Simple and Accurate Computations of Solvatochromic Shifts in $\pi \rightarrow \pi^*$ Transitions of Aromatic Chromophores. Journal of the American Chemical Society, 2001, 123, 11229-11236.	13.7	21
117	Normal and defective perylene substitution sites in alkane crystals. Journal of Chemical Physics, 2001, 114, 3224-3235.	3.0	15