

Hendrik Heinz

List of Publications by Year in descending order

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117
papers

9,333
citations

43973

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39575

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125
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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 12\AA^6 and 9\AA^6 Lennard-Jones Potentials. <i>Journal of Physical Chemistry C</i> , 2008, 112, 17281-17290.	1.5	792
2	Thermodynamically Consistent Force Fields for the Assembly of Inorganic, Organic, and Biological Nanostructures: The INTERFACE Force Field. <i>Langmuir</i> , 2013, 29, 1754-1765.	1.6	699
3	Nanoparticle decoration with surfactants: Molecular interactions, assembly, and applications. <i>Surface Science Reports</i> , 2017, 72, 1-58.	3.8	419
4	Force Field and a Surface Model Database for Silica to Simulate Interfacial Properties in Atomic Resolution. <i>Chemistry of Materials</i> , 2014, 26, 2647-2658.	3.2	369
5	Chemistry of Aqueous Silica Nanoparticle Surfaces and the Mechanism of Selective Peptide Adsorption. <i>Journal of the American Chemical Society</i> , 2012, 134, 6244-6256.	6.6	349
6	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.	6.6	334
7	Force Field for Mica-Type Silicates and Dynamics of Octadecylammonium Chains Grafted to Montmorillonite. <i>Chemistry of Materials</i> , 2005, 17, 5658-5669.	3.2	297
8	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.	3.2	248
9	Molecular models and simulations of layered materials. <i>Journal of Materials Chemistry</i> , 2009, 19, 2470.	6.7	244
10	Observing crystal nucleation in four dimensions using atomic electron tomography. <i>Nature</i> , 2019, 570, 500-503.	13.7	219
11	Atomic Charges for Classical Simulations of Polar Systems. <i>Journal of Physical Chemistry B</i> , 2004, 108, 18341-18352.	1.2	204
12	: A force field database for cementitious materials including validations, applications and opportunities. <i>Cement and Concrete Research</i> , 2017, 102, 68-89.	4.6	186
13	Adsorption mechanism of single amino acid and surfactant molecules to Au {111} surfaces in aqueous solution: design rules for metal-binding molecules. <i>Soft Matter</i> , 2011, 7, 2113.	1.2	185
14	Simulations of inorganic-bioorganic interfaces to discover new materials: insights, comparisons to experiment, challenges, and opportunities. <i>Chemical Society Reviews</i> , 2016, 45, 412-448.	18.7	176
15	Three-dimensional coordinates of individual atoms in materials revealed by electron tomography. <i>Nature Materials</i> , 2015, 14, 1099-1103.	13.3	172
16	Structure and Phase Transitions of Alkyl Chains on Mica. <i>Journal of the American Chemical Society</i> , 2003, 125, 9500-9510.	6.6	164
17	Building two-dimensional materials one row at a time: Avoiding the nucleation barrier. <i>Science</i> , 2018, 362, 1135-1139.	6.0	155
18	Influence of aluminates on the hydration kinetics of tricalcium silicate. <i>Cement and Concrete Research</i> , 2017, 100, 245-262.	4.6	146

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19	Carbon Nanotube Dispersion in Solvents and Polymer Solutions: Mechanisms, Assembly, and Preferences. <i>ACS Nano</i> , 2017, 11, 12805-12816.	7.3	145
20	Force Field for Tricalcium Silicate and Insight into Nanoscale Properties: Cleavage, Initial Hydration, and Adsorption of Organic Molecules. <i>Journal of Physical Chemistry C</i> , 2013, 117, 10417-10432.	1.5	141
21	Accurate Force Field Parameters and pH Resolved Surface Models for Hydroxyapatite to Understand Structure, Mechanics, Hydration, and Biological Interfaces. <i>Journal of Physical Chemistry C</i> , 2016, 120, 4975-4992.	1.5	139
22	Prediction of Specific Biomolecule Adsorption on Silica Surfaces as a Function of pH and Particle Size. <i>Chemistry of Materials</i> , 2014, 26, 5725-5734.	3.2	125
23	Insight into induced charges at metal surfaces and biointerfaces using a polarizable Lennard-Jones potential. <i>Nature Communications</i> , 2018, 9, 716.	5.8	121
24	Interaction energy and surface reconstruction between sheets of layered silicates. <i>Journal of Chemical Physics</i> , 2006, 124, 224713.	1.2	113
25	Tailoring Molecular Specificity Toward a Crystal Facet: a Lesson From Biorecognition Toward Pt{111}. <i>Nano Letters</i> , 2013, 13, 840-846.	4.5	101
26	Crystallographic Recognition Controls Peptide Binding for Bio-Based Nanomaterials. <i>Journal of the American Chemical Society</i> , 2011, 133, 12346-12349.	6.6	96
27	Elucidation of Peptide-Directed Palladium Surface Structure for Biologically Tunable Nanocatalysts. <i>ACS Nano</i> , 2015, 9, 5082-5092.	7.3	96
28	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.	3.2	95
29	Relation between Packing Density and Thermal Transitions of Alkyl Chains on Layered Silicate and Metal Surfaces. <i>Langmuir</i> , 2008, 24, 3727-3733.	1.6	94
30	Single- and multi-component chiral supraparticles as modular enantioselective catalysts. <i>Nature Communications</i> , 2019, 10, 4826.	5.8	93
31	Influence of the Shape of Nanostructured Metal Surfaces on Adsorption of Single Peptide Molecules in Aqueous Solution. <i>Small</i> , 2012, 8, 1049-1059.	5.2	92
32	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.	1.3	87
33	A force field for tricalcium aluminate to characterize surface properties, initial hydration, and organically modified interfaces in atomic resolution. <i>Dalton Transactions</i> , 2014, 43, 10602-10616.	1.6	87
34	Exploiting Localized Surface Binding Effects to Enhance the Catalytic Reactivity of Peptide-Capped Nanoparticles. <i>Journal of the American Chemical Society</i> , 2013, 135, 11048-11054.	6.6	86
35	Toward Understanding Amino Acid Adsorption at Metallic Interfaces: A Density Functional Theory Study. <i>ACS Applied Materials & Interfaces</i> , 2009, 1, 388-392.	4.0	85
36	Photoisomerization of Azobenzene Grafted to Layered Silicates: Simulation and Experimental Challenges. <i>Chemistry of Materials</i> , 2008, 20, 6444-6456.	3.2	82

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37	Clay minerals for nanocomposites and biotechnology: surface modification, dynamics and responses to stimuli. <i>Clay Minerals</i> , 2012, 47, 205-230.	0.2	81
38	Facet Recognition and Molecular Ordering of Ionic Liquids on Metal Surfaces. <i>Journal of Physical Chemistry C</i> , 2013, 117, 25969-25981.	1.5	80
39	Surface Structure of Organoclays. <i>Angewandte Chemie - International Edition</i> , 2004, 43, 2239-2243.	7.2	76
40	Calculation of local pressure tensors in systems with many-body interactions. <i>Physical Review E</i> , 2005, 72, 066704.	0.8	66
41	Polarization at metal-biomolecular interfaces in solution. <i>Journal of the Royal Society Interface</i> , 2011, 8, 220-232.	1.5	66
42	Molecular Mechanism of Specific Recognition of Cubic Pt Nanocrystals by Peptides and of the Concentration-Dependent Formation from Seed Crystals. <i>Advanced Functional Materials</i> , 2015, 25, 1374-1384.	7.8	65
43	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.	1.5	64
44	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.	3.8	59
45	Bending of Layered Silicates on the Nanometer Scale: Mechanism, Stored Energy, and Curvature Limits. <i>Journal of Physical Chemistry C</i> , 2011, 115, 22292-22300.	1.5	57
46	Stability, surface features, and atom leaching of palladium nanoparticles: toward prediction of catalytic functionality. <i>Physical Chemistry Chemical Physics</i> , 2013, 15, 5488.	1.3	57
47	Computational screening of biomolecular adsorption and self-assembly on nanoscale surfaces. <i>Journal of Computational Chemistry</i> , 2010, 31, 1564-1568.	1.5	56
48	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.	1.2	53
49	CHARMM-GUI Nanomaterial Modeler for Modeling and Simulation of Nanomaterial Systems. <i>Journal of Chemical Theory and Computation</i> , 2022, 18, 479-493.	2.3	53
50	A Rational Biomimetic Approach to Structure Defect Generation in Colloidal Nanocrystals. <i>ACS Nano</i> , 2014, 8, 6934-6944.	7.3	49
51	Atomic-scale identification of Pd leaching in nanoparticle catalyzed C-C coupling: effects of particle surface disorder. <i>Chemical Science</i> , 2015, 6, 6413-6419.	3.7	44
52	Peptide-Assisted 2-D Assembly toward Free-Floating Ultrathin Platinum Nanoplates as Effective Electrocatalysts. <i>Nano Letters</i> , 2019, 19, 3730-3736.	4.5	44
53	Involvement of prenucleation clusters in calcium phosphate mineralization of collagen. <i>Acta Biomaterialia</i> , 2021, 120, 213-223.	4.1	44
54	Direct correlation of oxygen adsorption on platinum-electrolyte interfaces with the activity in the oxygen reduction reaction. <i>Science Advances</i> , 2021, 7, .	4.7	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.	4.0	43
56	Atomic-Scale Structure and Stress Release Mechanism in Coreâ€“Shell Nanoparticles. ACS Nano, 2018, 12, 12296-12304.	7.3	41
57	Mechanism of molecular interaction of acrylate-polyethylene glycol acrylate copolymers with calcium silicate hydrate surfaces. Green Chemistry, 2020, 22, 1577-1593.	4.6	38
58	Molecular Dynamics Modeling of Epoxy Resins Using the Reactive Interface Force Field. Macromolecules, 2021, 54, 9815-9824.	2.2	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.	2.3	36
60	Force field for calcium sulfate minerals to predict structural, hydration, and interfacial properties. Cement and Concrete Research, 2021, 139, 106262.	4.6	35
61	Reliable computational design of biological-inorganic materials to the large nanometer scale using Interface-FF. Molecular Simulation, 2017, 43, 1394-1405.	0.9	34
62	Interpretable molecular models for molybdenum disulfide and insight into selective peptide recognition. Chemical Science, 2020, 11, 8708-8722.	3.7	32
63	Understanding the Surface Reactivity of Ligand-Protected Metal Nanoparticles for Biomass Upgrading. ACS Catalysis, 2020, 10, 5462-5474.	5.5	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.	1.5	31
65	Analysis of the phase transitions in alkyl-mica by density and pressure profiles. Journal of Chemical Physics, 2004, 120, 3847-3854.	1.2	30
66	Understanding Chemical Bonding in Alloys and the Representation in Atomistic Simulations. Journal of Physical Chemistry C, 2018, 122, 14996-15009.	1.5	30
67	Nature of peptide wrapping onto metal nanoparticle catalysts and driving forces for size control. Nanoscale, 2017, 9, 8401-8409.	2.8	29
68	Accurate simulation of surfaces and interfaces of ten FCC metals and steel using Lennardâ€“Jones potentials. Npj Computational Materials, 2021, 7, .	3.5	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.	3.8	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.	2.4	23
71	Calculation of local and average pressure tensors in molecular simulations. Molecular Simulation, 2007, 33, 747-758.	0.9	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.	0.7	23

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73	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.	1.5	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. <i>ACS Sustainable Chemistry and Engineering</i> , 2021, 9, 8354-8371.	3.2	22
75	Simple and Accurate Computations of Solvatochromic Shifts in $\pi \rightarrow \pi^*$ Transitions of Aromatic Chromophores. <i>Journal of the American Chemical Society</i> , 2001, 123, 11229-11236.	6.6	21
76	Long-Range Hierarchical Nanocrystal Assembly Driven by Molecular Structural Transformation. <i>Journal of the American Chemical Society</i> , 2019, 141, 1498-1505.	6.6	21
77	Energy-effective Grinding of Inorganic Solids Using Organic Additives. <i>Chimia</i> , 2017, 71, 451.	0.3	19
78	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.	7.8	19
79	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.	3.3	19
80	Control over Self-Assembly of Diblock Copolymers on Hexagonal and Square Templates for High Area Density Circuit Boards. <i>ACS Nano</i> , 2011, 5, 9413-9420.	7.3	18
81	Interactions at the Silica/Peptide Interface: Influence of the Extent of Functionalization on the Conformational Ensemble. <i>Langmuir</i> , 2018, 34, 8255-8263.	1.6	18
82	The role of chemistry and pH of solid surfaces for specific adsorption of biomolecules in solution – accurate computational models and experiment. <i>Journal of Physics Condensed Matter</i> , 2014, 26, 244105.	0.7	17
83	Enhancement of oxygen reduction reaction activity by grain boundaries in platinum nanostructures. <i>Nano Research</i> , 2020, 13, 3310-3314.	5.8	17
84	Vaporizable endoskeletal droplets via tunable interfacial melting transitions. <i>Science Advances</i> , 2020, 6, eaaz7188.	4.7	16
85	Cement Interfaces: Current Understanding, Challenges, and Opportunities. <i>Langmuir</i> , 2021, 37, 6347-6356.	1.6	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. <i>Journal of Colloid and Interface Science</i> , 2022, 605, 685-700.	5.0	16
87	Molecular modeling of chemical admixtures; opportunities and challenges. <i>Cement and Concrete Research</i> , 2022, 156, 106783.	4.6	16
88	Normal and defective perylene substitution sites in alkane crystals. <i>Journal of Chemical Physics</i> , 2001, 114, 3224-3235.	1.2	15
89	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.	1.8	14
90	Morphology of sulfonated polyarylenethioethersulfone random copolymer series as proton exchange fuel cells membranes by small angle neutron scattering. <i>Polymer</i> , 2011, 52, 5615-5621.	1.8	14

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91	Interaction of substituted poly(phenyleneethynylene)s with ligand-stabilized CdS nanoparticles. <i>Journal of Materials Chemistry A</i> , 2014, 2, 8705-8711.	5.2	13
92	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.	2.8	13
93	Molecular dynamics simulations of separator-cathode interfacial thermal transport in a Li-ion cell. <i>Surfaces and Interfaces</i> , 2020, 21, 100674.	1.5	11
94	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.	7.3	11
95	Furfuryl alcohol deoxygenation, decarbonylation, and ring-opening on Pt(111). <i>Surface Science</i> , 2018, 677, 333-340.	0.8	10
96	Single-shot 3D coherent diffractive imaging of core-shell nanoparticles with elemental specificity. <i>Scientific Reports</i> , 2018, 8, 8284.	1.6	10
97	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.	1.3	9
98	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.	2.4	7
99	Molecular structure and assembly of peptide-derived nanomaterials. <i>Current Opinion in Green and Sustainable Chemistry</i> , 2018, 12, 38-46.	3.2	6
100	Quantitative characterization of high temperature oxidation using electron tomography and energy-dispersive X-ray spectroscopy. <i>Scientific Reports</i> , 2018, 8, 10239.	1.6	6
101	Reactive modeling of Mo ₃ Si oxidation and resulting silica morphology. <i>Acta Materialia</i> , 2020, 187, 93-102.	3.8	6
102	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.	1.2	5
103	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.	1.2	5
104	Post-synthetic modification of ionic liquids using ligand-exchange and redox coordination chemistry. <i>Journal of Materials Chemistry A</i> , 2020, 8, 22674-22685.	5.2	5
105	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.	1.5	4
106	Adsorption and Diffusion of Oxygen on Pure and Partially Oxidized Metal Surfaces in Ultrahigh Resolution. <i>Nano Letters</i> , 2022, 22, 5392-5400.	4.5	4
107	UV-Absorption and Silica/Titania Colloids Using a Core-Shell Approach. <i>Silicon</i> , 2010, 2, 95-104.	1.8	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. <i>Journal of Physical Chemistry B</i> , 2017, 121, 1158-1167.	1.2	2

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109	Binding of polar and hydrophobic molecules at the LiCoO ₂ (001)-water interface: force field development and molecular dynamics simulations. <i>Nanoscale</i> , 2022, , .	2.8	2
110	Multiscale Experiments and Modeling in Biomaterials and Biological Materials, Part I. <i>Jom</i> , 2021, 73, 1673-1675.	0.9	1
111	Surface patterning in alloys. , 2022, 1, 103-104.		1
112	Three-Dimensional Determination of the Coordinates of Individual Atoms in Materials. <i>Microscopy and Microanalysis</i> , 2016, 22, 916-917.	0.2	0
113	4D Atomic Electron Tomography. <i>Microscopy and Microanalysis</i> , 2019, 25, 1814-1815.	0.2	0
114	Imaging Nucleation, Growth and Disorder at the Single-atom Level by Atomic Electron Tomography (AET). <i>Microscopy and Microanalysis</i> , 2020, 26, 1848-1850.	0.2	0
115	Multiscale Experiments and Modeling in Biomaterials and Biological Materials, Part II. <i>Jom</i> , 2021, 73, 2332-2334.	0.9	0
116	Anchoring of a hydrophobic heptapeptide (AFILPTG) on silica facilitates peptide unfolding at the abioticâ€“biotic interface. <i>Physical Chemistry Chemical Physics</i> , 2021, 23, 18001-18011.	1.3	0
117	Understanding Molecular Recognition on Metallic and Oxidic Nanostructures from a Perspective of Computer Simulation and Theory. , 2014, , 141-171.		0