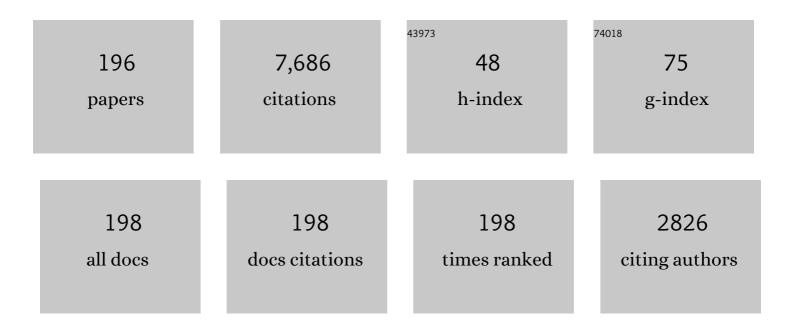
List of Publications by Year in descending order

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Πονοεμικί Ηου

#	Article	IF	CITATIONS
1	Reactive molecular dynamics and experimental study of graphene-cement composites: Structure, dynamics and reinforcement mechanisms. Carbon, 2017, 115, 188-208.	5.4	301
2	Calcium silicate hydrate from dry to saturated state: Structure, dynamics and mechanical properties. Acta Materialia, 2014, 67, 81-94.	3.8	241
3	Molecular dynamics modeling of the structure, dynamics, energetics and mechanical properties of cement-polymer nanocomposite. Composites Part B: Engineering, 2019, 162, 433-444.	5.9	231
4	Mechanism of cement paste reinforced by graphene oxide/carbon nanotubes composites with enhanced mechanical properties. RSC Advances, 2015, 5, 100598-100605.	1.7	206
5	Reactive Molecular Simulation on Water Confined in the Nanopores of the Calcium Silicate Hydrate Gel: Structure, Reactivity, and Mechanical Properties. Journal of Physical Chemistry C, 2015, 119, 1346-1358.	1.5	194
6	Molecular Dynamics Study on the Structure and Dynamics of NaCl Solution Transport in the Nanometer Channel of CASH Gel. ACS Sustainable Chemistry and Engineering, 2018, 6, 9498-9509.	3.2	172
7	Optimized design of ultra-high performance concrete (UHPC) with a high wet packing density. Cement and Concrete Research, 2019, 126, 105921.	4.6	151
8	Mechanical properties of calcium silicate hydrate (C–S–H) at nano-scale: A molecular dynamics study. Materials Chemistry and Physics, 2014, 146, 503-511.	2.0	146
9	Molecular dynamics study of water and ions transport in nano-pore of layered structure: A case study of tobermorite. Microporous and Mesoporous Materials, 2014, 195, 9-20.	2.2	141
10	Modified Lucas-Washburn function of capillary transport in the calcium silicate hydrate gel pore: A coarse-grained molecular dynamics study. Cement and Concrete Research, 2020, 136, 106166.	4.6	126
11	Chloride ions transport and adsorption in the nano-pores of silicate calcium hydrate: Experimental and molecular dynamics studies. Construction and Building Materials, 2016, 126, 991-1001.	3.2	108
12	Sustainable use of red mud in ultra-high performance concrete (UHPC): Design and performance evaluation. Cement and Concrete Composites, 2021, 115, 103862.	4.6	108
13	Effects of graphene oxide on the properties and microstructures of the magnesium potassium phosphate cement paste. Construction and Building Materials, 2016, 119, 107-112.	3.2	106
14	Interfacial Connection Mechanisms in Calcium–Silicate–Hydrates/Polymer Nanocomposites: A Molecular Dynamics Study. ACS Applied Materials & Interfaces, 2017, 9, 41014-41025.	4.0	106
15	Experimental and molecular dynamics studies on the transport and adsorption of chloride ions in the nano-pores of calcium silicate phase: The influence of calcium to silicate ratios. Microporous and Mesoporous Materials, 2018, 255, 23-35.	2.2	105
16	Comparative evaluation on the dispersion and stability of graphene oxide in water and cement pore solution by incorporating silica fume. Cement and Concrete Composites, 2018, 94, 33-42.	4.6	96
17	Two-scale modeling of transport properties of cement paste: Formation factor, electrical conductivity and chloride diffusivity. Computational Materials Science, 2015, 110, 270-280.	1.4	95
18	Uniaxial tension study of calcium silicate hydrate (C–S–H): structure, dynamics and mechanical properties. Materials and Structures/Materiaux Et Constructions, 2015, 48, 3811-3824.	1.3	84

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19	Water and chloride ions migration in porous cementitious materials: An experimental and molecular dynamics investigation. Cement and Concrete Research, 2017, 102, 161-174.	4.6	83
20	Reactive force field simulation on polymerization and hydrolytic reactions in calcium aluminate silicate hydrate (C–A–S–H) gel: structure, dynamics and mechanical properties. RSC Advances, 2015, 5, 448-461.	1.7	78
21	Water transport in the nano-pore of the calcium silicate phase: reactivity, structure and dynamics. Physical Chemistry Chemical Physics, 2015, 17, 1411-1423.	1.3	75
22	Experimental and computational investigation of magnesium phosphate cement mortar. Construction and Building Materials, 2016, 112, 331-342.	3.2	75
23	Nanoscale mechanism of ions immobilized by the geopolymer: A molecular dynamics study. Journal of Nuclear Materials, 2020, 528, 151841.	1.3	74
24	Reactive force-field molecular dynamics study on graphene oxide reinforced cement composite: functional group de-protonation, interfacial bonding and strengthening mechanism. Physical Chemistry Chemical Physics, 2018, 20, 8773-8789.	1.3	72
25	Combine ingress of chloride and carbonation in marine-exposed concrete under unsaturated environment: A numerical study. Ocean Engineering, 2019, 189, 106350.	1.9	72
26	Numerical study of carbonation and its effect on chloride binding in concrete. Cement and Concrete Composites, 2019, 104, 103402.	4.6	69
27	Molecular Dynamics Study of Water and Ions Transported during the Nanopore Calcium Silicate Phase: Case Study of Jennite. Journal of Materials in Civil Engineering, 2014, 26, 930-940.	1.3	67
28	Molecular dynamics simulation study on interfacial shear strength between calcium-silicate-hydrate and polymer fibers. Construction and Building Materials, 2020, 257, 119557.	3.2	67
29	Insights on the capillary transport mechanism in the sustainable cement hydrate impregnated with graphene oxide and epoxy composite. Composites Part B: Engineering, 2019, 173, 106907.	5.9	66
30	Two-scale modeling of the capillary network in hydrated cement paste. Construction and Building Materials, 2014, 64, 11-21.	3.2	65
31	Micro-mechanical properties of calcium sulfoaluminate cement and the correlation with microstructures. Cement and Concrete Composites, 2017, 80, 10-16.	4.6	64
32	Unraveling disadhesion mechanism of epoxy/CSH interface under aggressive conditions. Cement and Concrete Research, 2021, 146, 106489.	4.6	62
33	Molecular dynamics study on the chemical bound, physical adsorbed and ultra-confined water molecules in the nano-pore of calcium silicate hydrate. Construction and Building Materials, 2017, 151, 563-574.	3.2	61
34	Transport Properties of Sulfate and Chloride Ions Confined between Calcium Silicate Hydrate Surfaces: A Molecular Dynamics Study. Journal of Physical Chemistry C, 2018, 122, 28021-28032.	1.5	60
35	Molecular dynamics study on the mode I fracture of calcium silicate hydrate under tensile loading. Engineering Fracture Mechanics, 2014, 131, 557-569.	2.0	59
36	Insight on the mechanism of sulfate attacking on the cement paste with granulated blast furnace slag: An experimental and molecular dynamics study. Construction and Building Materials, 2018, 169, 601-611.	3.2	58

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37	Tuning interfacial structure and mechanical properties of graphene oxide sheets/polymer nanocomposites by controlling functional groups of polymer. Applied Surface Science, 2020, 504, 144152.	3.1	58
38	Morphology of calcium silicate hydrate (C-S-H) gel: a molecular dynamic study. Advances in Cement Research, 2015, 27, 135-146.	0.7	56
39	Cement-based material modified by in-situ polymerization: From experiments to molecular dynamics investigation. Composites Part B: Engineering, 2020, 194, 108036.	5.9	56
40	Effect of environmental pH values on phase composition and microstructure of Portland cement paste under sulfate attack. Composites Part B: Engineering, 2021, 216, 108862.	5.9	55
41	Estimate the relative electrical conductivity of C–S–H gel from experimental results. Construction and Building Materials, 2014, 71, 392-396.	3.2	54
42	Insights into the interfacial strengthening mechanisms of calcium-silicate-hydrate/polymer nanocomposites. Physical Chemistry Chemical Physics, 2018, 20, 8247-8266.	1.3	53
43	Theoretical investigation of epoxy detachment from C-S-H interface under aggressive environment. Construction and Building Materials, 2020, 264, 120232.	3.2	53
44	Preparation and mechanism of graphene oxide/isobutyltriethoxysilane composite emulsion and its effects on waterproof performance of concrete. Construction and Building Materials, 2019, 208, 343-349.	3.2	52
45	Molecular dynamics simulation of the interfacial bonding properties between graphene oxide and calcium silicate hydrate. Construction and Building Materials, 2020, 260, 119927.	3.2	51
46	Experimental and molecular modeling of polyethylene fiber/cement interface strengthened by graphene oxide. Cement and Concrete Composites, 2020, 112, 103676.	4.6	51
47	Molecular simulation of "hydrolytic weakening― A case study on silica. Acta Materialia, 2014, 80, 264-277.	3.8	50
48	External sulfate attack to reinforced concrete under drying-wetting cycles and loading condition: Numerical simulation and experimental validation by ultrasonic array method. Construction and Building Materials, 2017, 139, 365-373.	3.2	50
49	The effect of water molecules on the structure, dynamics, and mechanical properties of sodium aluminosilicate hydrate (NASH) gel: A molecular dynamics study. Construction and Building Materials, 2018, 193, 491-500.	3.2	50
50	Molecular structure, dynamics, and mechanical behavior of sodium aluminosilicate hydrate (NASH) gel at elevated temperature: a molecular dynamics study. Physical Chemistry Chemical Physics, 2018, 20, 20695-20711.	1.3	49
51	Insights into the interfacial strengthening mechanism of waste rubber/cement paste using polyvinyl alcohol: Experimental and molecular dynamics study. Cement and Concrete Composites, 2020, 114, 103791.	4.6	49
52	Superhydrophobic anticorrosive coating for concrete through in-situ bionic induction and gradient mineralization. Construction and Building Materials, 2020, 257, 119510.	3.2	49
53	A preliminary investigation of the properties of potassium magnesium phosphate cement-based grouts mixed with fly ash, water glass and bentonite. Construction and Building Materials, 2020, 237, 117501.	3.2	48
54	Application of neutron radiography in observing and quantifying the time-dependent moisture distributions in multi-cracked cement-based composites. Cement and Concrete Composites, 2017, 78, 13-20.	4.6	47

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55	Insights on Capillary Adsorption of Aqueous Sodium Chloride Solution in the Nanometer Calcium Silicate Channel: A Molecular Dynamics Study. Journal of Physical Chemistry C, 2017, 121, 13786-13797.	1.5	47
56	Fabrication of superhydrophobicity on foamed concrete surface by GO/silane coating. Materials Letters, 2020, 265, 127423.	1.3	47
57	Alkali-activated artificial aggregates fabricated by red mud and fly ash: Performance and microstructure. Construction and Building Materials, 2021, 281, 122552.	3.2	47
58	The mechanism of cesium ions immobilization in the nanometer channel of calcium silicate hydrate: a molecular dynamics study. Physical Chemistry Chemical Physics, 2017, 19, 27974-27986.	1.3	45
59	Microscopic insight into nanodiamond polymer composites: reinforcement, structural, and interaction properties. Nanoscale, 2020, 12, 24107-24118.	2.8	45
60	Insights on the molecular structure evolution for tricalcium silicate and slag composite: From 29Si and 27Al NMR to molecular dynamics. Composites Part B: Engineering, 2020, 202, 108401.	5.9	45
61	Nanoscale insight on the epoxy-cement interface in salt solution: A molecular dynamics study. Applied Surface Science, 2020, 509, 145322.	3.1	45
62	A novel Zn(<scp>ii</scp>) dithiocarbamate/ZnS nanocomposite for highly efficient Cr ⁶⁺ removal from aqueous solutions. RSC Advances, 2017, 7, 35075-35085.	1.7	44
63	Nano-scale mechanical properties investigation of C-S-H from hydrated tri-calcium silicate by nano-indentation and molecular dynamics simulation. Construction and Building Materials, 2018, 189, 265-275.	3.2	44
64	Molecular structure and dynamics of an aqueous sodium chloride solution in nano-pores between portlandite surfaces: a molecular dynamics study. Physical Chemistry Chemical Physics, 2016, 18, 2059-2069.	1.3	43
65	Confined Water Dissociation in Disordered Silicate Nanometer-Channels at Elevated Temperatures: Mechanism, Dynamics and Impact on Substrates. Langmuir, 2016, 32, 4153-4168.	1.6	42
66	Influence of aluminates on the structure and dynamics of water and ions in the nanometer channel of calcium silicate hydrate (C–S–H) gel. Physical Chemistry Chemical Physics, 2018, 20, 2373-2387.	1.3	41
67	Insights on magnesium and sulfate ions' adsorption on the surface of sodium alumino-silicate hydrate (NASH) gel: a molecular dynamics study. Physical Chemistry Chemical Physics, 2018, 20, 18297-18310.	1.3	41
68	Molecular dynamics study on the weakening effect of moisture content on graphene oxide reinforced cement composite. Chemical Physics Letters, 2018, 708, 177-182.	1.2	41
69	Compositions and microstructures of hardened cement paste with carbonation curing and further water curing. Construction and Building Materials, 2021, 267, 121724.	3.2	41
70	lonic hydration structure, dynamics and adsorption mechanism of sulfate and sodium ions in the surface of calcium silicate hydrate gel: A molecular dynamics study. Applied Surface Science, 2018, 448, 559-570.	3.1	40
71	Molecular dynamics study on ions and water confined in the nanometer channel of Friedel's salt: structure, dynamics and interfacial interaction. Physical Chemistry Chemical Physics, 2018, 20, 27049-27058.	1.3	40
72	Atomistic insights into cesium chloride solution transport through the ultra-confined calcium–silicate–hydrate channel. Physical Chemistry Chemical Physics, 2019, 21, 11892-11902.	1.3	40

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73	Design of sustainable ultra-high performance concrete: A review. Construction and Building Materials, 2021, 307, 124643.	3.2	40
74	RSM-based modelling and optimization of magnesium phosphate cement-based rapid-repair materials. Construction and Building Materials, 2020, 263, 120190.	3.2	39
75	Molecular dynamics study of solvated aniline and ethylene glycol monomers confined in calcium silicate nanochannels: a case study of tobermorite. Physical Chemistry Chemical Physics, 2017, 19, 15145-15159.	1.3	37
76	Molecular insight into the fluidity of cement pastes: Nano-boundary lubrication of cementitious materials. Construction and Building Materials, 2022, 316, 125800.	3.2	37
77	Calcite crystallization in the cement system: morphological diversity, growth mechanism and shape evolution. Physical Chemistry Chemical Physics, 2018, 20, 14174-14181.	1.3	36
78	Structure, Dynamics, and Mechanical Properties of Cross-Linked Calcium Aluminosilicate Hydrate: A Molecular Dynamics Study. ACS Sustainable Chemistry and Engineering, 2018, 6, 9403-9417.	3.2	36
79	Reactive molecular simulation on the ordered crystal and disordered glass of the calcium silicate hydrate gel. Ceramics International, 2016, 42, 4333-4346.	2.3	34
80	A reactive molecular dynamics study of graphene oxide sheets in different saturated states: structure, reactivity and mechanical properties. Physical Chemistry Chemical Physics, 2018, 20, 11053-11066.	1.3	34
81	Characterization of sustainable ultra-high performance concrete (UHPC) including expanded perlite. Construction and Building Materials, 2021, 303, 124245.	3.2	34
82	Insights into the molecular structure and reinforcement mechanism of the hydrogel-cement nanocomposite: An experimental and molecular dynamics study. Composites Part B: Engineering, 2019, 177, 107421.	5.9	33
83	Structural, dynamic and mechanical evolution of water confined in the nanopores of disordered calcium silicate sheets. Microfluidics and Nanofluidics, 2015, 19, 1309-1323.	1.0	31
84	Modification of incorporation and in-situ polymerization of aniline on the nano-structure and meso-structure of calcium silicate hydrates. Construction and Building Materials, 2018, 182, 459-468.	3.2	31
85	Na and Cl immobilization by size controlled calcium silicate hydrate nanometer pores. Construction and Building Materials, 2019, 202, 622-635.	3.2	31
86	Unraveling the microstructural properties of cement-slag composite pastes incorporated with smart polymer-based corrosion inhibitors: From experiment to molecular dynamics. Cement and Concrete Composites, 2022, 125, 104298.	4.6	31
87	Electrochemical chloride extraction (ECE) based on the high performance conductive cement-based composite anode. Construction and Building Materials, 2018, 173, 149-159.	3.2	29
88	Experimental and computational study on chloride ion transport and corrosion inhibition mechanism of rubber concrete. Construction and Building Materials, 2021, 268, 121105.	3.2	29
89	Insights on the adhesive properties and debonding mechanism of CFRP/concrete interface under sulfate environment: From experiments to molecular dynamics. Construction and Building Materials, 2021, 269, 121247.	3.2	29
90	Comprehensive performances of carbon nanotube reinforced foam concrete with tetraethyl orthosilicate impregnation. Construction and Building Materials, 2017, 131, 512-516.	3.2	28

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91	Molecular dynamics study on calcium silicate hydrate subjected to tension loading and water attack: structural evolution, dynamics degradation and reactivity mechanism. Physical Chemistry Chemical Physics, 2018, 20, 11130-11144.	1.3	27
92	Experiment and molecular dynamics study on the mechanism for hydrophobic impregnation in cement-based materials: A case of octadecane carboxylic acid. Construction and Building Materials, 2019, 229, 116871.	3.2	27
93	Experimental and molecular dynamics studies on the durability of sustainable cement-based composites: Reinforced by graphene. Construction and Building Materials, 2020, 257, 119566.	3.2	27
94	Silane Coupling Agent Modification Treatment to Improve the Properties of Rubber–Cement Composites. ACS Sustainable Chemistry and Engineering, 2021, 9, 12899-12911.	3.2	27
95	Insights on molecular structure and micro-properties of alkali-activated slag materials: A reactive molecular dynamics study. Construction and Building Materials, 2017, 139, 430-437.	3.2	26
96	Reactive molecular simulation on the calcium silicate hydrates/polyethylene glycol composites. Chemical Physics Letters, 2017, 687, 184-187.	1.2	26
97	Characterization of the corrosion profiles of reinforcement with different impressed current densities by X-ray micro-computed tomography. Cement and Concrete Composites, 2020, 109, 103583.	4.6	26
98	Enhancing interfacial bonding between epoxy and CSH using graphene oxide: An atomistic investigation. Applied Surface Science, 2021, 568, 150896.	3.1	26
99	Molecular Simulation of the Ions Ultraconfined in the Nanometer-Channel of Calcium Silicate Hydrate: Hydration Mechanism, Dynamic Properties, and Influence on the Cohesive Strength. Inorganic Chemistry, 2017, 56, 1881-1896.	1.9	25
100	Molecular dynamics study on the Tri-calcium silicate hydration in sodium sulfate solution: Interface structure, dynamics and dissolution mechanism. Construction and Building Materials, 2018, 170, 402-417.	3.2	24
101	Hydrophobic silane coating films for the inhibition of water ingress into the nanometer pore of calcium silicate hydrate gels. Physical Chemistry Chemical Physics, 2019, 21, 19026-19038.	1.3	24
102	Molecular dynamics study on sodium chloride solution transport through the Calcium-Silicate-Hydrate nanocone channel. Construction and Building Materials, 2022, 342, 128068.	3.2	24
103	Hydration for the Alite mineral: Morphology evolution, reaction mechanism and the compositional influences. Construction and Building Materials, 2017, 155, 413-426.	3.2	23
104	The effect of mechanical load on transport property and pore structure of alkali-activated slag concrete. Construction and Building Materials, 2018, 189, 397-408.	3.2	23
105	Molecular dynamics study onwater and ions on the surface of graphene oxide sheet: Effects of functional groups. Computational Materials Science, 2019, 167, 237-247.	1.4	23
106	Insight on the sodium and chloride ions adsorption mechanism on the ettringite crystal: Structure, dynamics and interfacial interaction. Computational Materials Science, 2018, 153, 479-492.	1.4	22
107	Protective Mechanism of Silane on Concrete upon Marine Exposure. Coatings, 2019, 9, 558.	1.2	22
108	Concentration-induced wettability alteration of nanoscale NaCl solution droplets on the CSH surface. Physical Chemistry Chemical Physics, 2021, 23, 7449-7461.	1.3	22

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109	Mesoscale insights on the structure, mechanical performances and the damage process of calcium-silicate-hydrate. Construction and Building Materials, 2021, 287, 123031.	3.2	22
110	Investigation of composite silane emulsion modified by in-situ functionalized graphene oxide for cement-based materials. Construction and Building Materials, 2021, 304, 124662.	3.2	22
111	Performance cement-based composite obtained by in-situ growth of organic–inorganic frameworks during the cement hydration. Construction and Building Materials, 2022, 336, 127533.	3.2	22
112	Nanoscale insights on the interface between passive film of steel and cement hydrate: Diffusion, kinetics and mechanics. Applied Surface Science, 2020, 514, 145898.	3.1	21
113	The design and evaluation of a smart polymer-based fluids transport inhibitor. Journal of Cleaner Production, 2020, 257, 120528.	4.6	21
114	Molecular insight in the wetting behavior of nanoscale water droplet on CSH surface: Effects of Ca/Si ratio. Applied Surface Science, 2022, 587, 152811.	3.1	21
115	Functionalization enhancement interfacial bonding strength between graphene sheets and calcium silicate hydrate: Insights from molecular dynamics simulation. Construction and Building Materials, 2020, 261, 120500.	3.2	20
116	Effects of water and ions on bonding behavior between epoxy and hydrated calcium silicate: a molecular dynamics simulation study. Journal of Materials Science, 2021, 56, 16475-16490.	1.7	20
117	Multi-scale study water and ions transport in the cement-based materials:from molecular dynamics to random walk. Microporous and Mesoporous Materials, 2021, 325, 111330.	2.2	20
118	Effect of sulfate attack on the composition and micro-mechanical properties of C-A-S-H gel in cement-slag paste: A combined study of nanoindentation and SEM-EDS. Construction and Building Materials, 2022, 345, 128275.	3.2	20
119	Structure, reactivity and mechanical properties of water ultra-confined in the ordered crystal: A case study of jennite. Microporous and Mesoporous Materials, 2015, 204, 106-114.	2.2	19
120	The inhibiting effect and mechanisms of smart polymers on the transport of fluids throughout nano-channels. Applied Surface Science, 2020, 500, 144019.	3.1	19
121	Synthesis, microstructure and mechanical properties of tricalcium phosphate–hydroxyapatite (TCP/HA) composite ceramic. Ceramics International, 2020, 46, 9810-9816.	2.3	19
122	Water distribution characteristics in cement paste with capillary absorption. Construction and Building Materials, 2020, 240, 117767.	3.2	19
123	Molecular dynamics study on ultra-confined NaCl solution in the silane coupling agent modified rubber calcium silicate hydrate nano-pore. Construction and Building Materials, 2021, 270, 121418.	3.2	19
124	Research and application progress of nano-modified coating in improving the durability of cement-based materials. Progress in Organic Coatings, 2021, 161, 106529.	1.9	19
125	Molecular dynamics study on calcium aluminosilicate hydrate at elevated temperatures: Structure, dynamics and mechanical properties. Materials Chemistry and Physics, 2019, 233, 276-287.	2.0	18
126	Structure, dynamics and mechanical properties evolution of calcium silicate hydrate induced by dehydration and dehydroxylation. Construction and Building Materials, 2021, 291, 123327.	3.2	18

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127	Insight on the nanoscale chemical degradation mechanism of MgCl2 attack in cement paste. Construction and Building Materials, 2020, 238, 117777.	3.2	17
128	Characterization of fly ash-cement paste and molecular structure in the presence of seawater by 27Al and 29Si MAS NMR spectroscopy. Construction and Building Materials, 2020, 262, 120823.	3.2	17
129	Insights into vitamin B3, B6 and C as inhibitor of steel reinforcement: A DFTÂ+ÂU study. Construction and Building Materials, 2021, 294, 123571.	3.2	17
130	Microscale peridynamic simulation of damage process of hydrated cement paste subjected to tension. Construction and Building Materials, 2019, 228, 117053.	3.2	16
131	Visualized tracing of capillary absorption process in cementitious material based on X ray computed tomography. Cement and Concrete Composites, 2020, 107, 103487.	4.6	16
132	The corrosion deterioration of reinforced passivation Film: The impact of defects. Applied Surface Science, 2022, 582, 152408.	3.1	16
133	Molecular Simulation of Calcium Silicate Composites: Structure, Dynamics, and Mechanical Properties. Journal of the American Ceramic Society, 2015, 98, 758-769.	1.9	15
134	Molecular structure, dynamics and adsorption behavior of water molecules and ions on [0â€ ⁻ 1â€ ⁻ 0] surface of γ-FeOOH: A molecular dynamics approach. Construction and Building Materials, 2019, 224, 785-795.	3.2	15
135	Effect of SiO2 Sol/Silane Emulsion in Reducing Water and Chloride Ion Penetration in Concrete. Coatings, 2020, 10, 682.	1.2	15
136	Insights on failure modes of calcium-silicate-hydrate interface strengthened by polyacrylamides: Structure, dynamic and mechanical properties. Construction and Building Materials, 2021, 278, 122406.	3.2	15
137	Preparation and characterization of an expanded perlite/paraffin/graphene oxide composite with enhanced thermal conductivity and leakage-bearing properties. RSC Advances, 2015, 5, 107514-107521.	1.7	14
138	Precipitated calcium hydroxide morphology in nanoparticle suspensions: An experimental and molecular dynamics study. Cement and Concrete Composites, 2018, 94, 201-214.	4.6	14
139	Microstructural Evolution Mechanism of C-(A)-S-H Gel in Portland Cement Pastes Affected by Sulfate Ions. Journal Wuhan University of Technology, Materials Science Edition, 2018, 33, 639-647.	0.4	14
140	Recyclable rubber-cement composites produced by interfacial strengthened strategy from polyvinyl alcohol. Construction and Building Materials, 2020, 264, 120541.	3.2	14
141	Influence of a New Type of Graphene Oxide/Silane Composite Emulsion on the Permeability Resistance of Damaged Concrete. Coatings, 2021, 11, 208.	1.2	14
142	Atypical adsorption of polycarboxylate superplasticizers on calcium silicate hydrate surface: Converting interaction by solvent effects. Construction and Building Materials, 2022, 330, 127160.	3.2	14
143	Large-scale simulation of calcium silicate hydrate by molecular dynamics. Advances in Cement Research, 2015, 27, 278-288.	0.7	13
144	A novel microporous amorphous-ZnO@TiO ₂ /graphene ternary nanocomposite with enhanced photocatalytic activity. RSC Advances, 2017, 7, 36787-36792.	1.7	13

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145	Insights on ions migration in the nanometer channel of calcium silicate hydrate under external electric field. Electrochimica Acta, 2019, 320, 134637.	2.6	13
146	Study on Unsaturated Transport of Cement-Based Silane Sol Coating Materials. Coatings, 2019, 9, 427.	1.2	13
147	Insights on the ion migration throughout the nano-channel of ettringite under an external electric field: Structure, dynamics, and mechanisms. Construction and Building Materials, 2020, 262, 120074.	3.2	13
148	Freezing mechanism of NaCl solution ultra-confined on surface of calcium-silicate-hydrate: A molecular dynamics study. Cement and Concrete Research, 2022, 154, 106722.	4.6	13
149	Bond behaviour between steel bar and concrete under sustained load and dry–wet cycles. Magazine of Concrete Research, 2019, 71, 700-709.	0.9	12
150	Water Transport Mechanisms of Poly(acrylic acid), Poly(vinyl alcohol), and Poly(ethylene glycol) in C–S–H Nanochannels: A Molecular Dynamics Study. Journal of Physical Chemistry B, 2020, 124, 6095-6104.	1.2	12
151	Strength and hydration attributes of cement pastes containing nano titania and cenosphere. Advances in Cement Research, 2020, 32, 557-572.	0.7	12
152	Nanoscale insight on the initial hydration mechanism of magnesium phosphate cement. Construction and Building Materials, 2021, 276, 122213.	3.2	12
153	Molecular dynamics study on water and ions transport mechanism in nanometer channel of 13X zeolite. Chemical Engineering Journal, 2021, 420, 129975.	6.6	12
154	Nanoscale insights into the anti-erosion performance of concrete: A molecular dynamics study. Applied Surface Science, 2022, 593, 153403.	3.1	12
155	Effect of magnesium on the C-S-H nanostructure evolution and aluminate phases transition in cement-slag blend. Journal Wuhan University of Technology, Materials Science Edition, 2018, 33, 108-116.	0.4	11
156	Experimentally validated peridynamic fracture modelling of mortar at the meso-scale. Construction and Building Materials, 2021, 267, 120939.	3.2	11
157	Molecular dynamics study the structure, bonding, dynamic and mechanical properties of calcium silicate hydrate with ultra-confined water: Effects of nanopore size. Construction and Building Materials, 2021, 280, 122477.	3.2	11
158	Evaluation and regulation of Ultra-High Performance Concrete (UHPC) crack resistance based on physicochemical multi-factor coupling approach. Construction and Building Materials, 2021, 301, 124100.	3.2	11
159	Molecular dynamics simulation of calcium silicate hydrate/tannic acid interfacial interactions at different temperatures: configuration, structure and dynamic. Construction and Building Materials, 2022, 326, 126820.	3.2	11
160	Load transfer mechanism at the calcium silicate hydrate/carbon nanotubes interface changed by carbon nanotubes surface modification investigated from atomic simulation. Applied Surface Science, 2022, 594, 153487.	3.1	11
161	A preliminary study of the properties of potassium phosphate magnesium cement-based grouts admixed with metakaolin, sodium silicate and bentonite. Construction and Building Materials, 2020, 262, 119893.	3.2	10
162	The Effect of Water Repellent Surface Impregnation on Durability of Cement-Based Materials. Advances in Materials Science and Engineering, 2017, 2017, 1-9.	1.0	9

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163	Basic properties and mechanism of high activity phosphate-based slurry for dynamic water blocking-A feasibility research. Construction and Building Materials, 2021, 275, 122040.	3.2	9
164	The unification of light weight and ultra-high strength in LWC: A new homogeneity enhancement approach. Construction and Building Materials, 2022, 315, 125647.	3.2	9
165	Understanding the wetting discrepancy in calcium alumino silicate hydrate induced by Al/Si ratio. Physical Chemistry Chemical Physics, 2022, 24, 6973-6987.	1.3	9
166	Influence of Cu Doping on the Hydration of Dicalcium Silicate: A First-Principles Study. ACS Sustainable Chemistry and Engineering, 2022, 10, 8094-8104.	3.2	9
167	Molecular Modeling of Capillary Transport in the Nanometer Pore of Nanocomposite of Cement Hydrate and Graphene/GO. Journal of Physical Chemistry C, 2019, 123, 15557-15568.	1.5	8
168	Effects of internally introduced sulfate on early age concrete properties: Active acoustic monitoring and molecular dynamics simulation. Construction and Building Materials, 2018, 188, 1014-1024.	3.2	7
169	Structure, dynamics and transport behavior of migrating corrosion inhibitors on the surface of calcium silicate hydrate: a molecular dynamics study. Physical Chemistry Chemical Physics, 2021, 23, 3267-3280.	1.3	7
170	Molecular-scale insights on structure-efficiency relationship of silane-based waterproofing agents. Construction and Building Materials, 2022, 327, 126985.	3.2	7
171	Understanding the deformation mechanism and mechanical characteristics of cementitious mineral analogues from first principles and reactive force field molecular dynamics. Physical Chemistry Chemical Physics, 2018, 20, 13920-13933.	1.3	6
172	Preparation of Modified Silane Composite Emulsion and Its Effect on Surface Properties of Cement-Based Materials. Coatings, 2021, 11, 272.	1.2	6
173	Structure, dynamics and mechanical properties evolution of calcium-silicate-hydrate induced by Fe ions: A molecular dynamics study. Construction and Building Materials, 2021, 287, 122875.	3.2	6
174	Rapid visualization and quantification of water penetration into cement paste through cracks with X-ray imaging. Cement and Concrete Composites, 2022, 125, 104293.	4.6	6
175	Nanomodified Cement-Based Materials: Review (2015–2020) of Molecular Dynamics Studies. Journal of Materials in Civil Engineering, 2022, 34, .	1.3	6
176	Preparation of Heavyweight Ultra-high Performance Concrete Using Barite Sand and Titanium-rich Heavy Slag Sand. Journal Wuhan University of Technology, Materials Science Edition, 2021, 36, 644-652.	0.4	6
177	Polymer functional coatings modified by ZrPâ€based composites: Preparation and applications on marine concrete. Journal of Applied Polymer Science, 2022, 139, .	1.3	6
178	Formation and Structure of Inhibitive Molecular Film of Oxadiazole on Iron Surface. Journal of Physical Chemistry C, 2017, 121, 21420-21429.	1.5	5
179	Visual analysis for microscopic cracking propagation of rubberized concrete. Construction and Building Materials, 2020, 265, 120599.	3.2	5
180	Efficacy and mechanism of GO/IBTS coating against microbial fouling of concrete surfaces in marine tidal areas. Journal of Coatings Technology Research, 2022, 19, 875-885.	1.2	5

#	Article	IF	CITATIONS
181	Numerical Analysis and Optimization on Piezoelectric Properties of 0–3 Type Piezoelectric Cement-Based Materials with Interdigitated Electrodes. Applied Sciences (Switzerland), 2017, 7, 233.	1.3	4
182	Efficacy and mechanism of graphene oxide modified silane emulsions on waterproof performance of foamed concrete. Case Studies in Construction Materials, 2022, 16, e00908.	0.8	4
183	Piezoelectric and magnetoelectric behaviors of multifunctional cement-based laminated composites. Construction and Building Materials, 2018, 180, 334-341.	3.2	3
184	Effect of Stirrup Corrosion and Fire on Shear Behavior of Reinforced Concrete Beams. KSCE Journal of Civil Engineering, 2021, 25, 3424-3436.	0.9	3
185	A molecular dynamics study of silicene reinforced cement composite at different humidity: Surface structure, bonding, and mechanical properties. Construction and Building Materials, 2021, 291, 123242.	3.2	3
186	Enhancement of Cement Paste with Carboxylated Carbon Nanotubes and Poly(vinyl alcohol). ACS Applied Nano Materials, 2022, 5, 6877-6889.	2.4	3
187	Nanoscale insight on the durability of magnesium phosphate cement: a molecular dynamics study. RSC Advances, 2020, 10, 40180-40195.	1.7	2
188	Temperature Effect of Hydration and Microstructure of Tricalcium Silicate–Slag Powder Hydrated Composites: An Experimental and Molecular Dynamics Investigation. ACS Sustainable Chemistry and Engineering, 2021, 9, 13773-13787.	3.2	2
189	Molecular Dynamics Study on Cement–Graphene Nanocomposite. , 2020, , 159-185.		1
190	Research on Preparation and Performance of Clay-Based Shield Tunnel Nonsintered Bricks. Advances in Materials Science and Engineering, 2021, 2021, 1-13.	1.0	1
191	Editorial: Molecular Simulation on Cementitious Materials: From Computational Chemistry Method to Application. Frontiers in Materials, 2021, 8, .	1.2	1
192	Modelling and Simulation for Concrete Durability: Mechanism and Prediction. Modelling and Simulation in Engineering, 2021, 2021, 1-2.	0.4	0
193	The Optimal Design on the Molecular Structure of a Fluid Transport Inhibitor Applied to Reinforced Concrete Structures. ACS Omega, 2021, 6, 29692-29702.	1.6	0
194	Molecular Simulation of Water and Ions Migration in the Nanometer Channel of Calcium Silicate Phase. , 2020, , 87-130.		0
195	Introduction to Modeling of Cement Hydrate at Nanoscale. , 2020, , 7-33.		0
196	Models for the Cross-Linked Calcium Aluminate Silicate Hydrate (C–A–S–H) Gel. , 2020, , 131-157.		0