Claire E White

List of Publications by Year
in descending order

75 papers	2,657 citations	218381 26 h-index	197535 49 g-index
75 all docs	75 docs citations	75 times ranked	2316 citing authors

#	Article	IF	Citations
1	X-ray microtomography shows pore structure and tortuosity in alkali-activated binders. Cement and Concrete Research, 2012, 42, 855-864.	4.6	394
2	Combining density functional theory (DFT) and pair distribution function (PDF) analysis to solve the structure of metastable materials: the case of metakaolin. Physical Chemistry Chemical Physics, 2010, 12, 3239.	1.3	137
3	The Effects of Temperature on the Local Structure of Metakaolinâ€Based Geopolymer Binder: A Neutron Pair Distribution Function Investigation. Journal of the American Ceramic Society, 2010, 93, 3486-3492.	1.9	135
4	Density Functional Modeling of the Local Structure of Kaolinite Subjected to Thermal Dehydroxylation. Journal of Physical Chemistry A, 2010, 114, 4988-4996.	1.1	113
5	Evolution of Local Structure in Geopolymer Gels: An <i>In Situ</i> Neutron Pair Distribution Function Analysis. Journal of the American Ceramic Society, 2011, 94, 3532-3539.	1.9	110
6	Mechanism of zinc oxide retardation in alkali-activated materials: an in situ X-ray pair distribution function investigation. Journal of Materials Chemistry A, 2017, 5, 11794-11804.	5.2	89
7	In situ synchrotron X-ray pair distribution function analysis of the early stages of gel formation in metakaolin-based geopolymers. Applied Clay Science, 2013, 73, 17-25.	2.6	82
8	Impact of chemical variability of ground granulated blast-furnace slag on the phase formation in alkali-activated slag pastes. Cement and Concrete Research, 2016, 89, 310-319.	4.6	82
9	In situ X-ray pair distribution function analysis of accelerated carbonation of a synthetic calciumâ€“silicateâ€“hydrate gel. Journal of Materials Chemistry A, 2015, 3, 8597-8605.	5.2	78
10	Intrinsic differences in atomic ordering of calcium (alumino)silicate hydrates in conventional and alkali-activated cements. Cement and Concrete Research, 2015, 67, 66-73.	4.6	72
11	Density functional modelling of silicate and aluminosilicate dimerisation solution chemistry. Dalton Transactions, 2011, 40, 1348-1355.	1.6	66
12	What Is the Structure of Kaolinite? Reconciling Theory and Experiment. Journal of Physical Chemistry B, 2009, 113, 6756-6765.	1.2	63
13	Molecular mechanisms responsible for the structural changes occurring during geopolymerization: Multiscale simulation. AICHE Journal, 2012, 58, 2241-2253.	1.8	60
14	In situ X-ray pair distribution function analysis of geopolymer gel nanostructure formation kinetics. Physical Chemistry Chemical Physics, 2013, 15, 8573.	1.3	60
15	Role of Magnesium-Stabilized Amorphous Calcium Carbonate in Mitigating the Extent of Carbonation in Alkali-Activated Slag. Chemistry of Materials, 2015, 27, 6625-6634.	3.2	52
16	Nanoscale Charge-Balancing Mechanism in Alkali-Substituted Calciumâ€“Silicateâ€“Hydrate Gels. Journal of Physical Chemistry Letters, 2016, 7, 5266-5272.	2.1	47
17	Alkali-activation of CaO-FeOx-SiO2 slag: Formation mechanism from in-situ X-ray total scattering. Cement and Concrete Research, 2019, 122, 179-188.	4.6	46
18	The effects of calcium hydroxide and activator chemistry on alkali-activated metakaolin pastes. Cement and Concrete Research, 2021, 145, 106453.	4.6	42

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19	Environmental stability of 2D anisotropic tellurium containing nanomaterials: anisotropic to isotropic transition. Nanoscale, 2017, 9, 12288-12294.	2.8	41
20	Molecular structure of CaOâ€"FeO_xâ€"SiO₂ glassy slags and resultant inorganic polymer binders. Journal of the American Ceramic Society, 2018, 101, 5846-5857.	1.9	40
21	Nanoscale Chemical Degradation Mechanisms of Sulfate Attack in Alkali-activated Slag. Journal of Physical Chemistry C, 2018, 122, 5992-6004.	1.5	37
22	Effect of Temperature on the Local Structure of Kaolinite Intercalated with Potassium Acetate. Chemistry of Materials, 2011, 23, 188-199.	3.2	33
23	Nanostructural characterization of geopolymers by advanced beamline techniques. Cement and Concrete Composites, 2013, 36, 56-64.	4.6	33
24	Nanoscale Ordering and Depolymerization of Calcium Silicate Hydrates in the Presence of Alkalis. Journal of Physical Chemistry C, 2019, 123, 24873-24883.	1.5	30
25	Amorphous nanoparticles by self-assembly: processing for controlled release of hydrophobic molecules. Soft Matter, 2019, 15, 2400-2410.	1.2	29
26	Quantitative Mechanistic Modeling of Silica Solubility and Precipitation during the Initial Period of Zeolite Synthesis. Journal of Physical Chemistry C, 2011, 115, 9879-9888.	1.5	28
27	Uncovering the True Atomic Structure of Disordered Materials: The Structure of a Hydrated Amorphous Magnesium Carbonate (MgCO₃Â·3D₂O). Chemistry of Materials, 2014, 26, 2693-2702.	3.2	26
28	Effects of temperature on the atomic structure of synthetic calciumâ€"silicateâ€"deuterate gels: A neutron pair distribution function investigation. Cement and Concrete Research, 2016, 79, 93-100.	4.6	26
29	Upscaling 3D Engineered Trees for Off-Grid Desalination. Environmental Science & Technology, 2022, 56, 1289-1299.	4.6	26
30	A parametric study of accelerated carbonation in alkali-activated slag. Cement and Concrete Research, 2021, 145, 106454.	4.6	25
31	Treatment of hydrogen background in bulk and nanocrystalline neutron total scattering experiments. Journal of Applied Crystallography, 2011, 44, 532-539.	1.9	24
32	Highly Surface-Active Ca(OH)₂ Monolayer as a CO₂ Capture Material. Nano Letters, 2018, 18, 1786-1793.	4.5	24
33	Spray drying OZ439 nanoparticles to form stable, water-dispersible powders for oral malaria therapy. Journal of Translational Medicine, 2019, 17, 97.	1.8	24
34	The use of XANES to clarify issues related to bonding environments in metakaolin: a discussion of the paper S. Sperinck et al., â€œDehydroxylation of kaolinite to metakaolin-a molecular dynamics study,â€• J. Mater. Chem., 2011, 21, 2118â€"2125. Journal of Materials Chemistry, 2011, 21, 7007.	6.7	23
35	A Roadmap for Production of Cement and Concrete with Low-CO2 Emissions. Waste and Biomass Valorization, 2021, 12, 4745-4775.	1.8	21
36	Evolution of the pore structure during the early stages of the alkali-activation reaction: an <i>in situ</i> small-angle neutron scattering investigation. Journal of Applied Crystallography, 2017, 50, 61-75.	1.9	20

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37	Impact of activator chemistry on permeability of alkaliâ€activated slags. Journal of the American Ceramic Society, 2017, 100, 4848-4859.	1.9	20
38	Rapid Recovery of Clofazimine-Loaded Nanoparticles with Long-Term Storage Stability as Anti-<i>Cryptosporidium</i> Therapy. ACS Applied Nano Materials, 2018, 1, 2184-2194.	2.4	20
39	<i>In situ</i> quasi-elastic neutron scattering study on the water dynamics and reaction mechanisms in alkali-activated slags. Physical Chemistry Chemical Physics, 2019, 21, 10277-10292.	1.3	20
40	Modeling of aqueous species interaction energies prior to nucleation in cement-based gel systems. Cement and Concrete Research, 2021, 139, 106266.	4.6	20
41	Multiscale pore structure determination of cement paste via simulation and experiment: The case of alkali-activated metakaolin. Cement and Concrete Research, 2020, 137, 106212.	4.6	19
42	Elucidating the atomic structures of different sources of fly ash using X-ray and neutron PDF analysis. Fuel, 2016, 177, 148-156.	3.4	18
43	Modeling Silica Nanoparticle Dissolution in TPAOHâˆ'TEOSâˆ'H2O Solutions. Journal of Physical Chemistry C, 2008, 112, 14769-14775.	1.5	16
44	Modeling the Formation of Alkali Aluminosilicate Gels at the Mesoscale Using Coarse-Grained Monte Carlo. Langmuir, 2016, 32, 11580-11590.	1.6	16
45	Effects of magnesium content and carbonation on the multiscale pore structure of alkali-activated slags. Cement and Concrete Research, 2020, 130, 105979.	4.6	16
46	Predicting CaO-(MgO)-Al2O3-SiO2 glass reactivity in alkaline environments from force field molecular dynamics simulations. Cement and Concrete Research, 2021, 150, 106588.	4.6	16
47	Selective Fluoride Transport in Subnanometer TiO₂ Pores. ACS Nano, 2021, 15, 16828-16838.	7.3	16
48	Novel Surface Molecular Functionalization Route To Enhance Environmental Stability of Tellurium-Containing 2D Layers. ACS Applied Materials & Interfaces, 2017, 9, 44625-44631.	4.0	15
49	Density functional modeling and total scattering analysis of the atomic structure of a quaternary<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:mi>CaO</mml:mi><mml:mtext>âˆ'</mml:mtext><mml:mi>M… mathvariant="normal">O</mml:mi><mml:mn>3</mml:mn></mml:msub><mml:mtext>âˆ'</mml:mtext><mml:msub><mml:mi>SiO</m… glass: Uncov. Physical Review Materials, 2021, 5, .	0.9	15
50	Inelastic neutron scattering analysis of the thermal decomposition of kaolinite to metakaolin. Chemical Physics, 2013, 427, 82-86.	0.9	14
51	Symmetry-Induced Stability in Alkali-Doped Calcium Silicate Hydrate. Journal of Physical Chemistry C, 2019, 123, 14081-14088.	1.5	13
52	Structure of kaolinite and influence of stacking faults: Reconciling theory and experiment using inelastic neutron scattering analysis. Journal of Chemical Physics, 2013, 138, 194501.	1.2	12
53	Physical Properties of Interfacial Layers Developed on Weathered Silicates: A Case Study Based on Labradorite Feldspar. Journal of Physical Chemistry C, 2019, 123, 24520-24532.	1.5	12
54	Pair distribution function analysis of amorphous geopolymer precursors and binders: the importance of complementary molecular simulations. Zeitschrift FÃ¼r Kristallographie, 2012, 227, 304-312.	1.1	11

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55	Anisotropic crystallization in solution processed chalcogenide thin film by linearly polarized laser. Applied Physics Letters, 2017, 110, .	1.5	11
56	Drying-induced atomic structural rearrangements in sodium-based calcium-alumino-silicate-hydrate gel and the mitigating effects of ZrO₂ nanoparticles. Physical Chemistry Chemical Physics, 2018, 20, 8593-8606.	1.3	11
57	The effects of calcium hydroxide and activator chemistry on alkali-activated metakaolin pastes exposed to high temperatures. Cement and Concrete Research, 2022, 154, 106742.	4.6	11
58	Comment on â€œStructure-Directing Role of Counterions in the Initial Stage of Zeolite Synthesisâ€• Journal of Physical Chemistry C, 2012, 116, 1619-1621.	1.5	10
59	Structure and properties of clay ceramics for thermal energy storage. Journal of the American Ceramic Society, 2017, 100, 4748-4759.	1.9	10
60	Extracting differential pair distribution functions using<i>MIXSCAT</i>. Journal of Applied Crystallography, 2010, 43, 635-638.	1.9	9
61	High-pressure polymorphism of<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:mi>Pb</mml:mi><mml:msub><mml:mi mathvariant="normal">F</mml:mi><mml:mn>2</mml:mn></mml:msub></mml:mrow></mml:math>to 75 GPa. Physical Review B, 2016, 94, .	1.1	9
62	Time-dependent phase quantification and local structure analysis of hydroxide-activated slag via X-ray total scattering and molecular modeling. Cement and Concrete Research, 2022, 151, 106642.	4.6	8
63	Nanoscale heterogeneities in a fractured alkali-activated slag binder: A helium ion microscopy analysis. Cement and Concrete Research, 2016, 79, 45-48.	4.6	7
64	Equation of state of the<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:mi>Î±</mml:mi><mml:mtext>â^'</mml:mtext><mml:mi>Pb</ mathvariant="normal">O</mml:mi><mml:mn>2</mml:mn></mml:msub></mml:mrow></mml:math>and<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:mi>P</mml:mi><mml:mi>a</mml:mi><mml:mover accent="true"><mml:mn>3</mml:mn><mml:mo>Â¯</mml:mo></mml:mover></mml:mrow></mml:math>-type phases of<mml:math xmlns:mml="http://www.w3.org/1998/. Physical Review B, 2018, 98, .	1.1	7
65	Ceramic Water Filters for the Removal of Bacterial, Chemical, and Viral Contaminants. Journal of Environmental Engineering, ASCE, 2019, 145, .	0.7	7
66	Removal Mechanisms of Contaminants in Ceramic Water Filters. Journal of Environmental Engineering, ASCE, 2018, 144, .	0.7	6
67	Chemoâ€mechanical properties of carbon fiber reinforced geopolymer interphase. Journal of the American Ceramic Society, 2022, 105, 1519-1532.	1.9	6
68	Discussion of Y. Zhang et al., â€œStudy of ion cluster reorientation process of geopolymerisation reaction using semi-empirical AM1 calculations,â€•Cem Concr Res 39(12): 1174â€"1179; 2009. Cement and Concrete Research, 2010, 40, 827-828.	4.6	4
69	A uniaxial load frame forin situneutron studies of stress-induced changes in cementitious materials and related systems. Review of Scientific Instruments, 2018, 89, 092903.	0.6	4
70	Understanding solution processing of inorganic materials using cryo-EM. Optical Materials Express, 2020, 10, 119.	1.6	3
71	Molecular Dynamics Simulations of Reverse Osmosis in Silica Nanopores. Journal of Physical Chemistry C, 2022, 126, 9161-9172.	1.5	3
72	Assessment of Ceramic Water Filters for the Removal of Bacterial, Chemical, and Viral Contaminants. Journal of Environmental Engineering, ASCE, 2020, 146, 04020066.	0.7	2

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73	Generic and Advanced Characterization Techniques. , 2020, , 31-497.		2
74	Accumulators for the Capture of Heavy Metals in Thermal Conversion Systems. Journal of Environmental Engineering, ASCE, 2018, 144, 04018118.	0.7	0
75	Solid Residues (Biochar, Bottom Ash, Fly Ash, â€¦). , 2020, , 1307-1387.		0