Journal of Neuromorphic Intelligence

PERSPECTIVE

VOLUME 03 | MARCH 2026

AI-driven Self-healing of Geopolymer Composite for Extreme Environments

Aolin Hou[1], Prashant Dhakal[2], Jingjing Qiu[3] ,Shiren Wang[1,2,*]

1 Department of Material Science and Engineering, Texas A&M University, College Station, TX, USA
2 Department of Industrial and Systems Engineering, Texas A&M University, College Station, TX, USA
3 Department of Mechanical Engineering, Texas A&M University, College Station, TX, USA
** Corresponding author: s.wang@tamu.edu*

ABSTRACT

Geopolymer composites are increasingly regarded as promising materials for infrastructure operating in extreme environments, including high-temperature, high-pressure, chemically aggressive, and multi-hazard conditions. However, passive durability alone is not sufficient to ensure long-term performance under such coupled extreme conditions. Once cracking occurs, transport pathways can rapidly form for fluids, ions, and reactive species, leading to permeability increase, loss of sealing integrity, structural degradation, and premature failure. This Perspective argues that the central challenge is therefore not simply to improve the intrinsic stability of geopolymers, but to design them for functional resilience through self-healing under coupled thermal, chemical, and pressure-driven stresses. We further contend that many current self-healing strategies remain overly generic and often fail to account for the distinct demands of different extreme environments. To address this gap, we propose a shift from empirical trial-and-error and forward property prediction toward physics-informed, mechanism-aware AI frameworks capable of inverse design, multimodal data integration, and digital-twin-assisted adaptation. Such an approach could enable geopolymer composites that are not only durable, but also damage-tolerant, recoverable, and better suited for long-term service in extreme environments.

Keywords: ***Extreme environments, Self-healing materials, Physics-informed AI, Digital twins***

1. THE CHALLENGE: EXTREME ENVIRONMENTS VS. CONVENTIONAL LOGIC

In the extreme environments relevant to deep geothermal and related subsurface applications, the central challenge extends beyond conventional durability as understood in ordinary civil engineering. Instead, the performance of construction materials is governed by the coupled action of thermal, chemical, and mechanical extremes, including high temperatures, elevated pressures, chemically aggressive brines, dissolved gases such as CO_2 and H_2S, and repeated thermo-mechanical loading. High-temperature geothermal wells are recognized as more demanding than typical oil and gas wells because they simultaneously expose materials to severe heat, corrosive chemical environments, and cyclic mechanical and thermal stresses (Figure 1a). In even more extreme conditions, superhot and supercritical geothermal systems may reach 500 °C, while supercritical geothermal fluids are commonly defined, for pure water, by temperatures above 374 °C and pressures above 22.1 MPa. Under these conditions, degradation processes of cementitious materials are markedly accelerated, and even minor cracks or interfacial defects can quickly

Received: 11 Janurary 2026

Accepted: 12 March 2026

Published: 23 March 2026

Check for updates

evolve into critical transport pathways for corrosive fluids, thereby compromising long-term integrity.[1-5].

The central flaw in conventional thinking is the tendency to regard material durability in extreme environments as a static, intrinsic property, rather than as a dynamic response that evolves under coupled damage, transport, and environmental attack. That assumption may be acceptable in mild service, but it breaks down in high-temperature, high-pressure, chemically aggressive environments where cracking accelerates transport and transport accelerates further degradation. The key scientific gap, therefore, is not whether construction materials possess sufficient initial strength and stability, but whether they can retain or recover functional resilience after damage under the specific stressors that drive failure in extreme environments.[6, 7]

1.1 THE DURABILITY GAP

Conventional cement remains structurally vulnerable in extreme geothermal service because its Ca-rich hydration products are susceptible to dehydration, decalcification, carbonation, and chemically assisted microstructural breakdown when heat, pressure, and aggressive fluids act together.[8] Recent geothermal well assessments show how quickly this becomes an integrity problem. The strength of ordinary Portland cement (OPC) samples decreased from 35 MPa to 5 MPa, experiencing a dramatic strength loss of 86% during the 9-month exposure in the well.[7] In other words, OPC fails not simply because it is exposed to elevated temperature, but because its intrinsic degradation pathways are strongly amplified by the coupled thermal, chemical, and pressure-driven transport conditions of the service environment.

Calcium Aluminate Cements (CAC)-based systems and thermal shock resistant cement (TSRC) represent important advances beyond OPC, particularly because they were developed to withstand high temperature, thermal shock, and chemically aggressive well conditions. CAC formulations have shown much better performance retention than OPC/silica blends during long-term geothermal exposure, while TSRC has demonstrated high thermal-shock resistance and substantial strength recovery after repeated heating-cooling cycles.[7, 9] However, they still largely represent optimized passive cement systems.

By contrast, geopolymer composites are a more promising long-term direction because their crosslinked aluminosilicate network provides a broader and more tunable platform for achieving low permeability, chemical stability, and adaptive sealing behavior under coupled thermal, chemical, and pressure-driven stresses in extreme conditions (Figure 1b).[6, 10, 11] However, these advantages should not be mistaken for true resilience. High-temperature exposure can drive shrinkage, densification, and microcracking in geopolymer networks,[12] while pressure-assisted fluid ingress can convert microstructural damage into sealing failure. In practice, the service life of a geothermal seal is seldom determined by the stability of the intact matrix alone; rather, it is ultimately governed by the initiation and propagation of cracks, debonding at interfaces, and the resulting evolution of permeability under sustained pressure and repeated thermal cycling. Consequently, the real durability gap lies in translating geopolymer stability to true resilience under extreme conditions.

1.2 THE RESILIENCE PARADOX

Although geopolymers often exhibit superior chemical resistance, many formulations remain susceptible to restrained shrinkage, early-age cracking, and localized brittle failure. Several studies have shown that alkali-activated slag and related systems can exhibit a markedly increased risk of cracking at high temperatures, especially when pore structure, activator chemistry, and curing history amplify capillary and autogenous stresses (Figure 2).[13-16] The implication is straightforward: the geopolymer composites can be highly durable in its intact state and still be a poor resilient material if it cannot limit crack opening or recover function once cracking occurs.

Self-healing research points toward a solution for permanent sealing capacity, particularly in demanding well environments, but much of the current literature is still too generic for truly extreme environments. In geopolymer systems, autogenous healing, microcapsule-based healing, bacteria-enabled healing, hollow fiber-assisted healing, shape memory materials (SMMs), superabsorbent polymers (SAPs), and mineral-forming additives have all shown promise, yet their effectiveness is highly conditional rather than universal. Reported healing efficiency depends strongly on crack width, water availability, activator chemistry, ionic composition, pH, and temperature.[14, 17, 18]. In addition, the healing subsystem itself may become the weak link: bacterial routes are constrained by high alkalinity, heat, and limited water availability, while SAPs-based and autogenous routes depend on fluid access, swelling behavior, and the continued formation

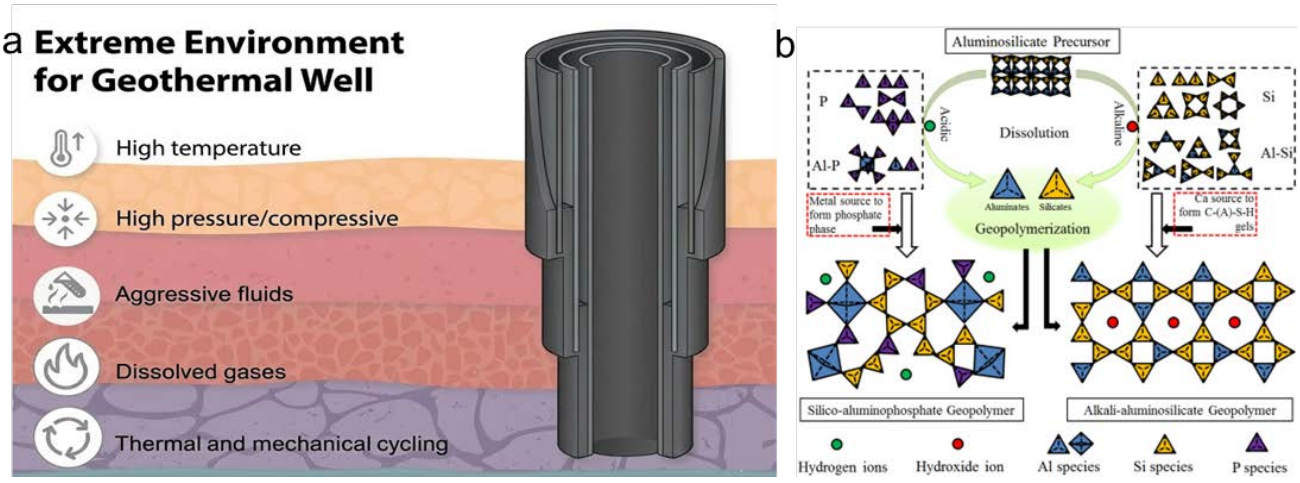


Figure 1: Illustration of (a) extreme environments for a geothermal well ,and (b) general geopolymerisation process[11] . Reprinted with permission,[11] open-access source (CC BY 4.0).

of stable sealing products. These dependencies already complicate healing under ambient or moderately aggressive conditions, and they become even more restrictive when the target environment shifts to geothermal service involving 375–500 °C exposure, high pressure, and corrosive alkaline or supercritical brines.

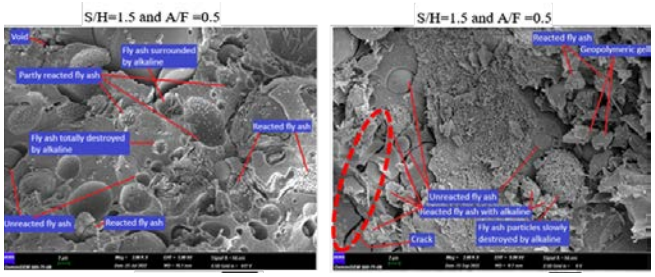


Figure 2: SEM images of Geopolymer with a 1.5 Na2SiO3/ NaOH ratio (S/H) and a 0.5 alkali activator /fly ash ratio (A/F) at 25 °C and 400 °C. Reprinted with permission16, open-access source (CC BY 4.0).

Under such conditions, a strategy that performs well in laboratory crack-closure tests may no longer preserve viability, activation, or product stability in service. For that reason, the design objective in extreme environments cannot be visual crack closure alone. The more meaningful target is recovery of transport resistance, interfacial integrity, and long-term sealing reliability under the same coupled thermal, chemical, and pressure conditions that generated the damage in the first place.

2. THE MISSING LINK: WHY AI?

Once the problem is framed around damage-specific resilience rather than generic strength, the design challenge becomes combinatorial. The choice space for manufacturing geopolymer composites already spans precursor chemistry, Si/Al balance, Ca content, activator type and dosage, liquid-to-solid ratio, fibers, fillers, curing route, and interfacial architecture. Adding a self-healing function multiplies that space again through bacteria, carriers, capsules, SMMs, SAPs, mineral additives, crack-width control strategies, and trigger conditions. Then the extreme conditions multiply it once more: H_2S-bearing brines, thermal cycling, sulfate or marine exposure, high pressure, fire, freeze-thaw, and supercritical water each favor different degradation and healing pathways. This is not a single-property optimization problem. It is a coupled search problem across chemistry, mechanism, and hazard profile.

2.1 COMPLEXITY OVERLOAD

Trial-and-error cannot navigate this space efficiently. Even when the target appears simple, such as maintaining strength after exposure to high temperature, the real objective is multidimensional: pumpability, set control, crack resistance, healing efficiency, permeability recovery, and long-term chemical stability must all be balanced. Machine learning has already begun to change how geopolymer are modeled, especially for property prediction and mixture optimization.[19, 20] But the deeper value of AI in this context is not only faster regression on the strength data. It is the ability to structure the design space, expose hidden variable interactions, and prioritize the next informative experiment under severe data and cost constraints.

This transition is critical as the multi-dimensional variables governing geopolymer design under extreme conditions, specifically the non-linear couplings



Figure 3: Approaches of self-healing for geopolymer composites.

between activator chemistry, shrinkage susceptibility, and healing kinetics, surpass the traditional boundaries of empirical intuition. AI will not replace the mechanistic understanding of materials. It is valuable here because the design space has become too large and complex for intuition alone to navigate effectively. What the field needs is not more isolated formulations, but a workflow that can learn from sparse heterogeneous datasets and direct experiments toward stressor-relevant regions of composition-mechanism space (Figure 3).[21]

2.2 FROM PREDICTION TO SYNTHESIS

Most current AI work in geopolymer materials is still framed as a forward problem: given a formulation, predict strength or another target property. While useful, this approach is not sufficient for self-healing geopolymers intended for extreme environments. The more relevant challenge is inverse design Given a defined stressor profile and a required recovery metric, what matrix chemistry and healing strategy should be selected to deliver the desired performance? For example, an H_2S-rich, high-pressure brine environment is unlikely to favor the same healing mechanism as repeated thermal cycling. The former is more likely to require chemically stable, non-biological healing chemistry together with dense, crack-limiting matrices, whereas the latter may benefit more from thermal-expansion matching, fiber-assisted crack control, and healing pathways that remain effective during repeated crack opening and closure. These considerations should not be treated as downstream implementation choices, but as defining elements of the design target itself. [19-22]

An actionable roadmap is now emerging for self-healing geopolymer composites designed for extreme environments (Figure 4).[22] First, the target exposure must be defined explicitly, including the relevant extreme-condition factors such as high temperature, high pressure, corrosive alkaline or supercritical fluids, thermal cycling, or H_2S-rich brines, together with the true failure criterion: permeability recovery, sealing retention, crack tolerance, or interface stability, rather than compressive-strength retention alone. Second, published data and new experiments should be organized into stressor-tagged datasets for self-healing geopolymer systems, rather than treated as generic composition–property tables. Third, the design space should be constrained using chemistry-informed descriptors, thermodynamic screening, and physical plausibility, so that only realistic matrix–healing combinations are explored. Fourth, surrogate models and active-learning workflows should be used to identify the most informative next experiments under defined extreme-service conditions. Fifth, inverse or generative design should be used to propose geopolymer formulations and healing architectures tailored to specific damage scenarios, rather than merely interpolating among known mixtures. Finally, the resulting candidates must be validated under realistic multi-hazard protocols that reproduce the same thermal, chemical, and pressure conditions that drive damage in service. Without this closed-loop framework, AI will simply accelerate rediscovery of ambient-condition trends.

However, the limitations are real and should not be hidden. Data scarcity is severe, especially for crack-sealing recovery under geothermal conditions. Reproducibility is weakened by inconsistent precursor reporting, incompatible healing metrics, and poor exposure standardization. Interpretability matters because safety-critical infrastructure cannot rely on opaque recommendations. Scale-up is also nontrivial: a lab-scale self-healing concept must still satisfy pumping, storage, trigger reliability, cost, and long-duration exposure requirements. But these are not arguments against AI-guided self-healing design. They are precisely the reasons the field needs a more disciplined, closed-loop, evidence-based design strategy.

3. THE NEW PERSPECTIVE — PHYSICS-INFORMED, MECHANISM-AWARE AI

Building on the durability and self-healing concepts introduced in the preceding sections, the central argument of this Perspective is that geopolymer design must move beyond correlation-based property prediction toward mechanism-aware AI. Current machine-learning studies in geopolymer research have been valuable for estimating compressive strength, mix proportions, and processing windows, but most remain trained on sparse, heterogeneous literature datasets and

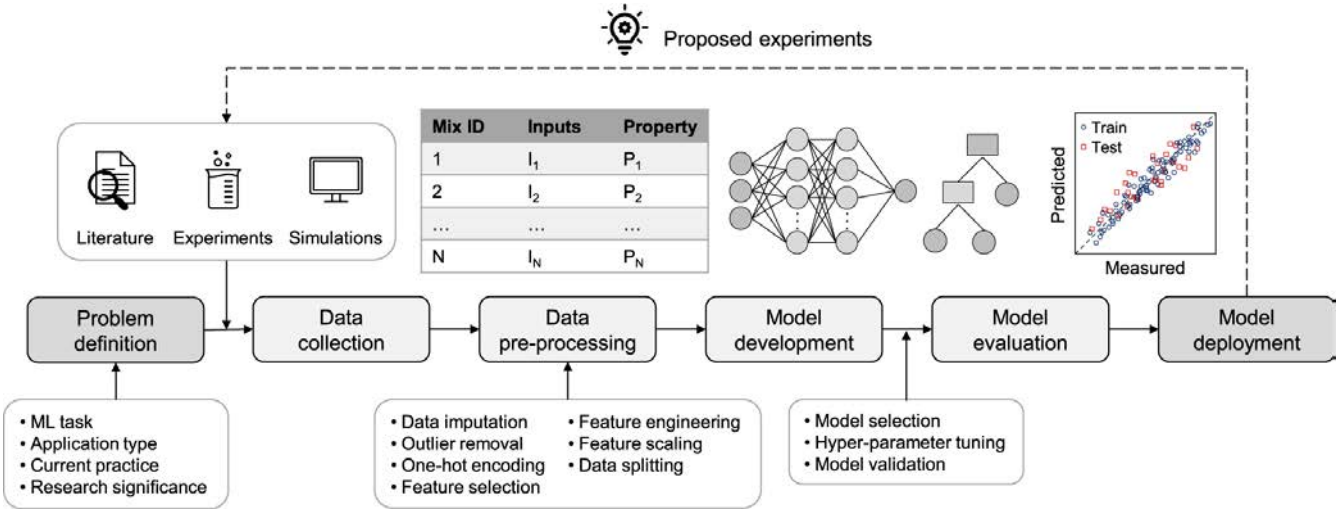


Figure 4: General workflow of machine learning (ML) in geopolymer science. Reprinted with permission,21 open-access source (CC BY 4.0).

are rarely structured around degradation, healing, or service-life adaptation under extreme environments. As a result, they are better at interpolation across known recipes than at reasoning about how a material should respond to thermal shock, acid or sulfate ingress, CO_2-rich subsurface exposure, or repeated pressurization cycles. [10, 23, 24]

The proposed shift is to couple data-driven learning with the chemistry and physics already known to govern alkali-activated systems[25]. In geopolymers, dissolution of aluminosilicate precursors, oligomer formation, polycondensation, pore-solution evolution, and temperature- and moisture-dependent transport jointly determine both mechanical integrity and healing capacity. A useful AI model should therefore embed chemical reaction kinetics, thermodynamic admissibility, and transport constraints rather than treat mix design as an unconstrained black box. PINNs offer a credible foundation for this direction because they can enforce governing equations during training, incorporate sparse experimental data, and infer latent state variables that are difficult to measure directly. For geopolymers, that means models in which reaction extent, gel formation, ionic transport, crack closure, and healing-product precipitation are learned together under physical constraints, rather than as isolated regression targets.[26-29]

In this framing, AI no longer merely predicts performance; it becomes a surrogate for coupled chemo-thermo-mechanical evolution. A mechanism-aware model could, for example, learn when a formulation that maximizes initial stiffness also amplifies thermal incompatibility, or when a matrix chemistry that improves acid resistance suppresses the mobility needed for autogenous or encapsulated healing. This is particularly important for geopolymers intended for fire-prone infrastructure, aggressive wastewater or marine exposure, and wellbore or geothermal service, where durability and recoverability are not independent objectives. The scientific opportunity is to recast the classic durability-resilience tradeoff as a dynamic co-optimization problem in which chemistry, pore architecture, healing strategy, and exposure history evolve together.[6, 30-32]

A second conceptual pivot is the digital twin. Rather than assuming that a geopolymer is fully characterized at the time of casting, a digital-twin framework treats the material and structure as continuously updated systems. Sensor streams from acoustic emission, distributed fiber optics, temperature and humidity probes, and related structural-health-monitoring modalities can be assimilated into a virtual replica that updates the internal damage state, healing state, and remaining performance margin in real time. For self-healing geopolymers, this is especially powerful because healing is inherently path-dependent: crack width, moisture availability, alkali mobility, reaction products, and repeated loading all influence whether recovery is partial, delayed, or sustained. A digital twin can therefore act as the bridge between laboratory understanding and field adaptation. [33-35]

The third pivot is multimodal integration within autonomous optimization loops. Future geopolymer discovery should not rely on one dataset type alone. Composition, precursor mineralogy, activator chemistry, curing profile, pore-network descriptors, spectroscopy, microscopy, mechanical response, durability trajectories, sensing time series, and even life-cycle carbon metrics should be fused into a single learning workflow. In adjacent areas of materials science, multimodal learning and self-driving laboratories are already showing how closed-loop experimentation can accelerate inverse design and multi-objective optimization. Applied to geopolymers, the analogous workflow would use mechanism-aware surrogates to propose candidate formulations, automated experiments to test them, digital twins to evaluate field-relevant adaptation, and optimization engines to update the next design cycle. The outcome is not just a stronger binder, but a geopolymer system that learns toward durability, recoverability, and sustainability simultaneously.[24, 36-38]

4. STRATEGIC ROADBLOCKS & THE PATH FORWARD

If Section 3 defines the conceptual architecture, the next question is what prevents its realization. The first roadblock is the data foundation itself. Geopolymer datasets remain fragmented across precursor classes, activator chemistries, curing schedules, specimen geometries, and test protocols. Most published databases emphasize early-age strength, while long-term durability, repeated damage-healing cycles, and sensor-rich exposure histories are rarely reported in a

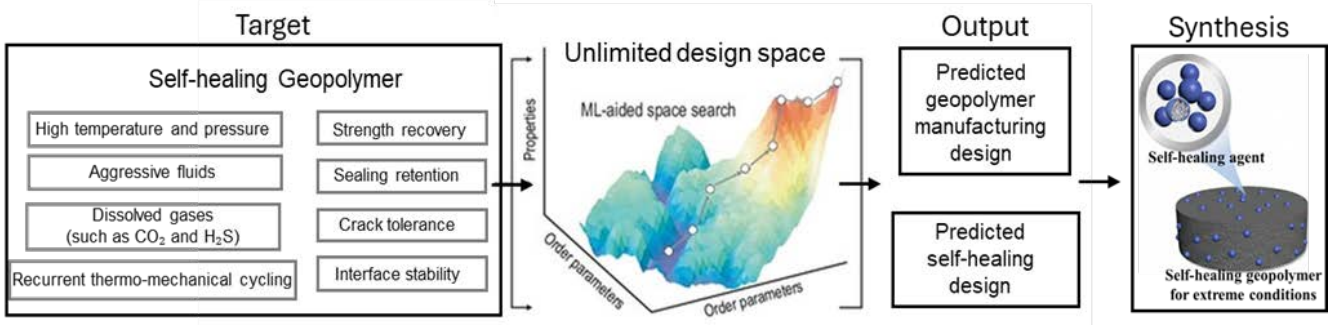


Figure 5: Inverse design as the conceptual bridge from target properties to candidate materials. Adopted with permission,[22] open-access source (CC BY 4.0).

standardized form. Self-healing studies are even more heterogeneous, often differing in crack-generation methods, healing duration, environmental conditions, and recovery metrics. Under these conditions, even sophisticated AI models risk learning publication artifacts rather than transferable mechanisms[10, 39, 40]
The second roadblock is mechanistic incompleteness. For mechanism-aware AI to be credible, geopolymer science must provide better state variables and constraints than bulk strength and porosity alone. What is needed are datasets and models that track reaction progress, gel chemistry, transport evolution, thermal incompatibility, crack morphology, and healing-product formation across time. Without these intermediate descriptors, AI cannot robustly distinguish whether failure was controlled by chemistry, transport, thermal mismatch, or interfacial instability. This is especially limiting in extreme environments, where high temperature, corrosive fluids, and confining pressure can re-order the dominant degradation pathway over time.[26 27, 30, 31]
The third roadblock is deployment. Digital twins for civil materials are advancing rapidly, but harsh-environment geopolymer applications require sensing systems that survive corrosion, thermal gradients, pressure cycling, and long maintenance intervals. Sensor survivability, calibration drift, bandwidth, and interoperability with materials databases remain unresolved barriers. Just as important, infrastructure owners will not adopt AI-guided materials without trustworthy uncertainty quantification, interpretable failure forecasts, and validation protocols that connect laboratory coupons to structural components and field assets. In other words, the challenge is not only model accuracy, but epistemic credibility.[33-35]
The path forward should therefore be strategic rather than incremental. First, the field needs benchmark datasets that jointly report precursor chemistry, activator composition, curing history, crack geometry, exposure protocol, sensor outputs, healing metrics, and embodied-carbon indicators in interoperable formats. Second, AI development should prioritize hybrid models that combine thermodynamic calculations, transport relations, and PINN-style constraints with active-learning experiments. Third, validation should be hierarchical: paste to mortar, mortar to concrete, concrete to element, and element to monitored pilot deployment. Fourth, optimization objectives must be explicitly multi-objective, balancing residual strength, permeability recovery, damage tolerance, cost, constructability, and life-cycle emissions. Framed this way, the research agenda becomes a coordinated platform for discovery rather than a collection of disconnected prediction studies.[24, 36, 41, 42]

5. CONCLUDING OUTLOOK

The most important implication of this Perspective is that the future of geopolymer research should not be defined by static property prediction alone. The field is ready to move from asking which formulation performs best under one prescribed test, to asking which self-healing strategy can sense damage, adapt its internal chemistry, recover function, and remain stable across evolving extremes. Physics-informed, mechanism-aware AI provides the intellectual framework for that transition because it connects first-principles understanding with real-time data, rather than forcing a choice between them. In that sense, self-healing geopolymers should be viewed not simply as alternative binders, but as candidate adaptive material systems.[28, 40, 41]
Looking ahead, the key goal is not simply to create substitutes for conventional cement, but to establish

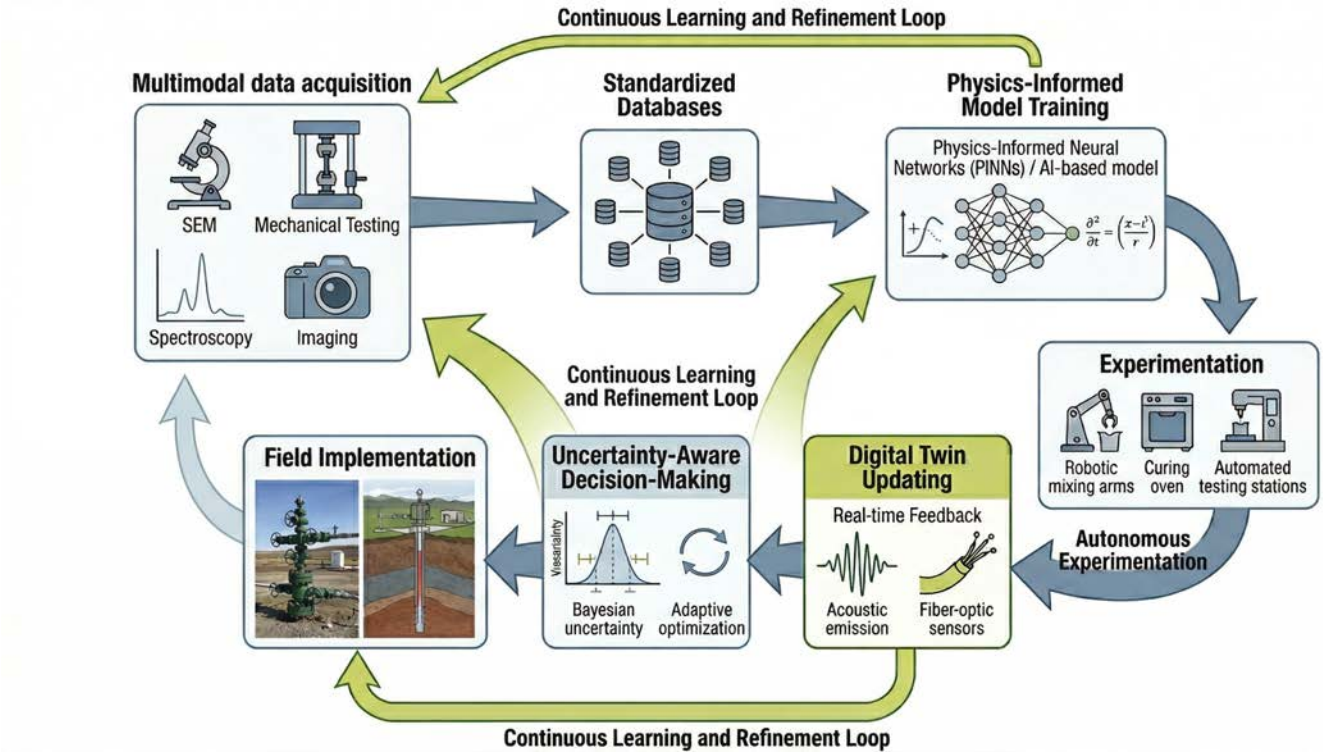


Figure 6: Roadmap for closed-loop deployment of self-healing geopolymers, showing standardized multimodal datasets, physics-informed model training, autonomous experimentation, digital-twin updating from acoustic emission and fiber-optic sensing, uncertainty-aware decision support, and translation to standards-ready field implementation.

geopolymer-based materials as resilient sealing systems for extreme environments. In geothermal and related subsurface applications, long-term performance will depend less on the stability of the intact matrix alone than on the ability to control cracking, preserve interface integrity, and restore sealing under coupled thermal, chemical, and pressure-driven stresses. Achieving this will require a shift from passive durability toward stressor-specific self-healing, supported by AI-guided design frameworks that can connect damage scenario, healing mechanism, and geopolymer chemistry in a targeted way. The real promise of AI-guided self-healing geopolymers is therefore not only better materials optimization, but a route toward more adaptive, resilient, and reliable infrastructure for extreme-service conditions.[6, 31, 41, 42]

REFRENCES

1. Duxson, P.; Fernández-Jiménez, A.; Provis, J. L.; Lukey, G. C.; Palomo, A.; van Deventer, J. S. J. Geopolymer technology: the current state of the art. Journal of Materials Science 2007, 42 (9), 2917-2933. DOI: 10.1007/s10853-006-0637-z.
2. Provis, J. L.; Bernal, S. A. Geopolymers and related alkali-activated materials. Annual review of materials research 2014, 44 (1), 299-327.
3. Provis, J. L. Alkali-activated materials. Cement and concrete research 2018, 114, 40-48.
4. Bakharev, T. Durability of geopolymer materials in sodium and magnesium sulfate solutions. Cement and concrete research 2005, 35
5. Bakharev, T. Resistance of geopolymer materials to acid attack. Cement and concrete research 2005, 35 (4), 658-670.
6. Wang, A.; Zheng, Y.; Zhang, Z.; Liu, K.; Li, Y.; Shi, L.; Sun, D. The durability of alkali-activated materials in comparison with ordinary Portland cements and concretes: a review. Engineering 2020, 6 (6), 695-706.
7. Pyatina, T.; Sugama, T.; Moghadam, A.; Naumann, M.; Skorpa, R.; Feneuil, B.; Soustelle, V.; Godøy, R. Assessment of cementitious composites for high-temperature geothermal wells. Materials 2024, 17 (6), 1320.
8. Kruszewski, M.; Wittig, V. Review of failure modes in supercritical geothermal drilling projects. Geothermal Energy 2018, 6 (1), 28
9. Sugama, T.; Pyatina, T. Hydrophobic Lightweight Cement with Thermal Shock Resistance and Thermal Insulating Properties for Energy-Storage Geothermal Well Systems. Materials 2021, 14 (21), 6679.
10. Wong, L. S. Durability Performance of Geopolymer Concrete: A Review. Polymers 2022, 14 (5), 868
11. Wang, Y. S.; Alrefaei, Y.; Dai, J. G. Silico-Aluminophosphate and Alkali-Aluminosilicate Geopolymers: A Comparative Review. Frontiers in Materials 2019, 6, Review. DOI: 10.3389/fmats.2019.00106
12. Krishna, R. S.; Mishra, S.; Sethy, N.; Mustakim, S. M.; Boopathy, R.; Rawat, S.; Qureshi, T. S. Impact of high-temperature exposure on the thermal and physio-mechanical performance of graphene-reinforced geopolymer composites. Construction and Building Materials 2025, 489, 142285. DOI: https://doi.org/10.1016/j.conbuildmat.2025.142285.
13. Khan, I.; Xu, T.; Castel, A.; Gilbert, R. I.; Babaee, M. Risk of early age cracking in geopolymer concrete due to restrained shrinkage. Construction and Building Materials 2019, 229, 116840.
14. Hammad, N.; Elnemr, A.; Shaaban, I. G. State-of-the-art report: the self-healing capability of alkali-activated slag (AAS) concrete. Materials 2023, 16 (12), 4394
15. Collins, F.; Sanjayan, J. G. Effect of pore size distribution on drying shrinking of alkali-activated slag concrete. Cement and Concrete Research 2000, 30 (9), 1401-1406
16. Kucukgoncu, H.; Özbayrak, A. Microstructural analysis of low-calcium fly ash-based geopolymer concrete with different ratios of activator and binder under high temperatures. Arabian Journal for Science and Engineering 2025, 50 (11), 8197-8223
17. Zhang, L. V.; Suleiman, A. R.; Allaf, M. M.; Marani, A.; Tuyan, M.; Nehdi, M. L. Crack self-healing in alkali-activated slag composites incorporating immobilized bacteria. Construction and Building Materials 2022, 326, 126842.
18. Yang, J.; Sun, Z.; De Belie, N.; Snoeck, D. Self-healing ability of cracks in alkali-activated slag systems incorporating superabsorbent polymers. Cement and Concrete Research 2023, 170, 107183
19. Zhang, L. V.; Marani, A.; Nehdi, M. L. Chemistry-informed machine learning prediction of compressive strength for alkali-activated materials. Construction and Building Materials 2022, 316, 126103
20. Ke, X.; Duan, Y. Coupling machine learning with thermodynamic modelling to develop a composition-property model for alkali-activated materials. Composites Part B: Engineering 2021, 216, 108801
21. Li, Z.; Yoon, J.; Zhang, R.; Rajabipour, F.; Srubar III, W. V.; Dabo, I.; Radlińska, A. Machine learning in concrete science: applications, challenges, and best practices. npj computational materials 2022, 8 (1), 127
22. Lu, S.; Zhou, Q.; Chen, X.; Song, Z.; Wang, J. Inverse design with deep generative models: next step in materials discovery. National science review 2022, 9 (8), nwac111
23. Hsu, C.-H.; Chan, H.-Y.; Chang, M.-H.; Liu, C.-F.; Liu, T.-Y.; Chiu, K.-C. Efficient compressive strength prediction of alkali-activated waste materials using machine learning. Materials 2024, 17 (13), 3141
24. Kong, Y.; Kurumisawa, K.; Tokoro, C.; Li, Z.; Chu, S. Data-driven inverse mix design for sustainable alkali-activated materials. Journal of Sustainable Cement-Based Materials 2024, 13 (12), 1857-1878
25. Dhakal, P.; Liu, R.; Kim, J. G.; Hou, A.; Wu, X.; Wang, S. Data-Efficient Machine Learning for in-situ Curing-aided Additive Manufacturing. Journal of Neuromorphic Intelligence 2024, 1 (1).
26. Provis, J. L. Geopolymers and other alkali activated materials: why, how, and what? Materials and structures 2014, 47 (1), 11-25
27. Provis, J. L.; Palomo, A.; Shi, C. Advances in understanding alkali-activated materials. Cement and Concrete Research 2015, 78, 110-125.
28. Raissi, M.; Perdikaris, P.; Karniadakis, G. E. Physics-informed neural networks: A deep learning framework for solving forward and inverse problems involving nonlinear partial differential equations. Journal of Computational physics 2019, 378, 686-707
29. Ji, W.; Qiu, W.; Shi, Z.; Pan, S.; Deng, S. Stiff-pinn: Physics-informed neural network for stiff chemical kinetics. The Journal of Physical Chemistry A 2021, 125 (36), 8098-8106.
30. Liu, Y.; Hu, X.; Du, Y.; Nematollahi, B.; Shi, C. A review on high-temperature resistance of geopolymer concrete. Journal of Building Engineering 2024, 98, 111241
31. Hajiabadi, S. H.; Khalifeh, M.; van Noort, R.; Silva Santos Moreira, P. H. Review on geopolymers as

wellbore sealants: state of the art optimization for CO2 exposure and perspectives. ACS omega 2023, 8 (26), 23320-23345
32. Borçato, A. G.; Medeiros-Junior, R. A. Self-healing in metakaolin-based geopolymers with crystalline admixture, expansive agent, and hydrated lime. Construction and Building Materials 2024, 418, 135391
33. Bado, M. F.; Tonelli, D.; Poli, F.; Zonta, D.; Casas, J. R. Digital twin for civil engineering systems: An exploratory review for distributed sensing updating. Sensors 2022, 22 (9), 3168.
34. Behnia, A.; Chai, H. K.; Shiotani, T. Advanced structural health monitoring of concrete structures with the aid of acoustic emission. Construction and building materials 2014, 65, 282-302.
35. Moser, D.; Martin-Candilejo, A.; Cueto-Felgueroso, L.; Santillán, D. Use of fiber-optic sensors to monitor concrete dams: recent breakthroughs and new opportunities. In Structures, 2024; Elsevier: Vol. 67, p 106968
36. Tom, G.; Schmid, S. P.; Baird, S. G.; Cao, Y.; Darvish, K.; Hao, H.; Lo, S.; Pablo-García, S.; Rajaonson, E. M.; Skreta, M. Self-driving laboratories for chemistry and materials science. Chemical Reviews 2024, 124 (16), 9633-9732
37. Wang, S.; Gong, S.; Böger, T.; Newnham, J. A.; Vivona, D.; Sokseiha, M.; Gordiz, K.; Aggarwal, A.; Zhu, T.; Zeier, W. G. Multimodal machine learning for materials science: Discovery of novel Li-ion solid electrolytes. Chemistry of Materials 2024, 36 (23), 11541-11550.
38. Wu, Y.; Ding, M.; He, H.; Wu, Q.; Jiang, S.; Zhang, P.; Ji, J. A versatile multimodal learning framework bridging multiscale knowledge for material design. npj Computational Materials 2025, 11 (1), 276.
39. Singh, B.; Ishwarya, G.; Gupta, M.; Bhattacharyya, S. Geopolymer concrete: A review of some recent developments. Construction and building materials 2015, 85, 78-90.
40. Al-Fakih, A.; Mahamood, M. A. A.; Al-Osta, M. A.; Ahmad, S. Performance and efficiency of self-healing geopolymer technologies: a review. Construction and Building Materials 2023, 386, 131571
41. Kriven, W. M.; Leonelli, C.; Provis, J. L.; Boccaccini, A. R.; Attwell, C.; Ducman, V. S.; Ferone, C.; Rossignol, S.; Luukkonen, T.; Van Deventer, J. S. Why geopolymers and alkali activated materials are key components of a sustainable world: A perspective contribution. Journal of the American ceramic society 2024, 107 (8), 5159-5177.
42. Martinez, A.; Miller, S. A. Life cycle assessment and production cost of geopolymer concrete: A meta-analysis. Resources, Conservation and Recycling 2025, 215, 108018.

COMPETING INTERESTS

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper

ACKNOWLEDGMENTS

The authors are grateful for the funding support from Texas A&M University