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AI-Based Analysis of EEG and Neuro-imaging Correlates of PCL-R Dimensions: Opportunities, Constraints, and a Research Agenda

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Abstract— *Psychopathy is conventionally assessed through structured clinical interviews and behavioral rating instruments such as the Psychopathy Checklist-Revised (PCL-R), a process that is time-intensive, dependent on rater training, and not scalable for large-cohort or screening use. Advances in electroencephalography (EEG) signal processing, functional magnetic resonance imaging (fMRI) analysis, and deep learning have enabled automated classification pipelines for a range of psychiatric and neurological conditions, raising the question of whether comparable pipelines could support research into the neurocognitive correlates of psychopathic traits. This paper does not report a trained model or empirical classification results; rather, it proposes a conceptual and methodological framework intended to orient future empirical work in this area. We review the current state of AI-assisted neuroimaging classification in adjacent psychiatric domains, identify the specific theoretical and practical obstacles that distinguish psychopathy research from those domains, and propose a four-layer framework spanning theoretical grounding, data and labeling strategy, computational modeling, and validation. We argue that the field's most useful near-term contribution is not a binary psychopath/non-psychopath classifier but a dimensional, explainable, cross-validated modeling approach anchored to established neurocognitive theory. We close with a concrete research agenda and an explicit discussion of the ethical constraints that should shape how such systems are built, evaluated, and reported.*

Keywords— psychopathy; EEG; fMRI; neuroimaging; deep learning; explainable AI; multimodal fusion; PCL-R; forensic neuroscience.

I. INTRODUCTION

Psychopathy is a personality construct characterized by a cluster of interpersonal, affective, lifestyle, and antisocial features, most commonly operationalized in research and forensic settings through the Hare Psychopathy Checklist-Revised (PCL-R), a 20-item instrument scored from a semi-structured interview and collateral file review. The PCL-R yields a continuous, dimensional score and can additionally support categorical diagnostic use above an established cutoff, though this cutoff varies by jurisdiction (typically 30 in North America, 25 in Europe for research purposes).

Because PCL-R administration requires trained clinical raters, extended interview time, and access to file information, it does not scale easily to large-sample research, and its scoring, while psychometrically well validated, retains an irreducible interpretive component. This has motivated interest in whether neurophysiological or neuroimaging signals could support, corroborate, or accelerate research into psychopathic traits. In parallel, AI-assisted classification from EEG and fMRI has matured substantially in adjacent psychiatric domains, including schizophrenia, depression, anxiety, bipolar disorder, and neurodevelopmental conditions, with systematic reviews now available for each of these areas.

This paper synthesizes that adjacent literature and translates its methodological lessons into a conceptual framework specifically for psychopathy-related neuroimaging research. Rather than proposing a single model architecture and reporting

simulated or assumed performance figures, we treat the framework itself as the contribution: a structured account of what a scientifically defensible, ethically bounded, and publishable research program in this space would need to contain.

1.1 Contribution of This Paper

- A synthesis of methodological lessons from AI-based EEG/fMRI classification in adjacent psychiatric domains, applied to the specific case of psychopathy research.
- Identification of the construct-validity and data-availability obstacles that make a naive binary-classification approach to psychopathy scientifically fragile.
- A four-layer conceptual framework (theoretical, data/labeling, computational, validation) intended to guide future empirical studies.
- A concrete, prioritized research agenda for groups with access to appropriate forensic or clinical cohorts.
- An explicit ethical framing for how such systems should and should not be used or reported.

II. RELATED WORK

2.1 AI-Based Classification from EEG in Psychiatric Research

Deep learning has been applied broadly to EEG-based psychiatric classification. A recent study trained deep learning models on resting-state quantitative EEG (power spectral density and functional connectivity across frequency bands) from a cohort of 945 individuals spanning six major and nine specific psychiatric disorder categories, illustrating both the feasibility and the scale that well-powered EEG classification studies now require [1]. Systematic reviews of EEG-based classification exist for schizophrenia [2], for obsessive-compulsive disorder [4], and for depression, anxiety, and bipolar disorder specifically [10], the last of which centers on explainable AI (XAI) methods such as SHAP and class activation mapping to identify which electrodes and frequency bands drive classification decisions, commonly implicating frontal and parietal sites and beta/alpha band activity depending on the disorder.

A recurring finding across these reviews is heterogeneity: study populations, preprocessing pipelines, validation strategies (many studies use within-dataset cross-validation rather than external replication), and reported accuracy vary widely, and few studies provide statistical or mechanistic interpretation of what their models have learned. The OCD-focused systematic review, for example, screened 42 studies and retained only 11 that met basic methodological inclusion criteria, citing exactly this heterogeneity as a barrier to clinical translation [4].

2.2 AI-Based Classification from fMRI and Multimodal Fusion

Parallel work in fMRI-based classification has applied convolutional neural networks, graph neural networks, and transformer-based architectures to resting-state and task fMRI for conditions including schizophrenia, autism spectrum disorder, and depression [7]. A widely cited systematic review and meta-analysis of deep learning applications for psychiatric disorder classification from neuroimaging data found that reported performance was often inflated by methodological weaknesses, including small sample sizes, information leakage between training and test sets, and insufficient external validation [8]. This caution generalizes directly to any future psychopathy-focused effort: reported accuracy figures in this literature should be treated skeptically unless cross-cohort generalization is demonstrated.

Multimodal fusion of imaging with other data streams, and attention-based fusion architectures specifically, have shown consistent gains in interpretability and, in several domains, accuracy, relative to single-modality models [11]. Explainable multimodal frameworks combining Grad-CAM-style saliency mapping with SHAP feature attribution have been used to align model decisions with domain-recognized biomarkers in radiology, dermatology, and audio-based diagnostic tasks, and represent a template that a psychopathy-focused framework can adopt: fusing modalities at an intermediate representational stage and requiring model attention to converge on theoretically predicted regions or features, rather than accepting attention patterns uncritically.

2.3 What Is Distinct About Psychopathy as a Target Construct

Two features distinguish psychopathy from the conditions reviewed above. First, unlike schizophrenia or depression, psychopathy is not a DSM/ICD diagnostic category; it is a dimensional personality construct assessed via the PCL-R or related instruments (e.g., the Psychopathic Personality Inventory-Revised, PPI-R), and the PCL-R itself is explicitly designed to

produce a dimensional score, with categorical use as a secondary application. Reviews of the PCL-R's predictive validity note that associations between psychopathy scores and external outcomes are broadly consistent across community, clinical, and forensic samples despite differing mean severity levels [5], [6], which supports dimensional modeling across heterogeneous populations rather than a single clinical-versus-healthy binary.

It is also important to note that the PCL-R comprises two correlated but distinct factors: Factor 1 (interpersonal/affective features, including grandiosity, manipulativeness, lack of empathy, and shallow affect) and Factor 2 (antisocial/lifestyle features, including impulsivity, irresponsibility, and antisocial behavior). These factors have been shown to have differential neurocognitive correlates; Factor 1 is more strongly associated with amygdala and ventromedial prefrontal cortex dysfunction, while Factor 2 shares variance with broader externalizing psychopathology [12], [13]. Any modeling approach that treats total PCL-R score as a unitary target risks obscuring these differential associations. A more informative strategy may be to predict factor scores separately or to explicitly model the factor structure.

Second, there is no equivalent to the large, open, multi-site EEG or fMRI repositories that exist for depression, schizophrenia, or Alzheimer's disease research. Psychopathy-relevant neuroimaging data has historically been collected in smaller forensic or offender cohorts, is not uniformly open-access, and carries additional consent, stigma, and data-sensitivity considerations given its association with criminal-justice contexts. Any realistic research program in this space must treat data access, not model architecture, as the primary bottleneck.

III. PROPOSED CONCEPTUAL FRAMEWORK

We propose a four-layer framework intended to keep future empirical work anchored to theory, honest about label quality, methodologically comparable to adjacent literature, and validated in a way that supports genuine generalization claims. The layers are sequential in development but should be revisited iteratively; a finding at the computational layer that fails to align with the theoretical layer should prompt a return to feature design rather than a search for a better classifier.

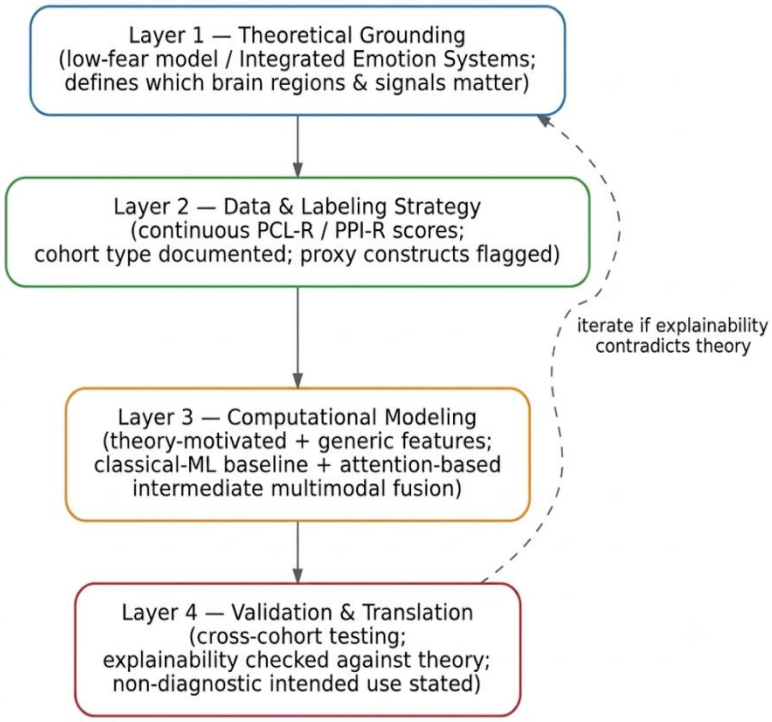

FIGURE 1: The proposed four-layer conceptual framework

3.1 Layer 1: Theoretical Grounding

Feature and hypothesis selection should be derived from an explicit neurocognitive theory rather than from whatever features are easiest to compute. Two influential accounts are the low-fear model, which attributes psychopathic traits to reduced amygdala reactivity to threat and distress cues, and the integrated emotion systems (IES) account, which frames psychopathy in terms of impaired stimulus-reinforcement learning and dysfunction in amygdala-orbitofrontal circuitry supporting moral and emotional decision-making [12], [13]. A theory-first approach constrains the feature space (e.g., prioritizing amygdala and

ventromedial prefrontal cortex activity in fMRI, or frontal theta/beta ratio and reduced frontal engagement in EEG) and gives any downstream explainability output something specific to be checked against.

3.2 Layer 2: Data and Labeling Strategy

We recommend three specific departures from the outline typically seen in early-stage proposals in this space:

1) **Use continuous PCL-R (or PPI-R) scores as the prediction target**, modeled as regression or ordinal classification, rather than a forced binary psychopath/non-psychopath label. This matches the instrument's intended use and avoids arbitrary cutoff effects. Where feasible, consider predicting Factor 1 and Factor 2 scores separately to capture differential neurocognitive associations.

2) **Where a validated forensic or clinical cohort with EEG/fMRI and PCL-R scores is not available**, use a proxy dimensional construct with existing open data, such as callous-unemotional traits or antisocial personality features, and state explicitly that findings are proxy-construct findings, not psychopathy findings, until validated on a PCL-R-scored sample.

3) **Report cohort composition (forensic, clinical, community), base rates, and comorbidities in detail**, since associations between psychopathy and external variables have been shown to hold across these settings but at different severity levels, and pooling them without accounting for this can distort model calibration.

3.3 Layer 3: Computational Modeling

Preprocessing and feature extraction should follow established pipelines: bandpass filtering, independent component analysis-based artifact removal (ocular, muscular) for EEG; standard motion correction, normalization, and parcellation for fMRI.

EEG Feature Recommendations:

Feature Category	Specific Features	Theoretical Basis
Resting-state power	Frontal theta/beta ratio, alpha asymmetry, delta/theta power	Reduced frontal engagement, abnormal inhibitory control
Event-related potentials	Reduced P300 amplitude, abnormal N400, reduced error-related negativity (ERN)	Impaired attention allocation, reduced error monitoring
Functional connectivity	Coherence, phase-locking value, directed transfer function	Disrupted fronto-limbic connectivity
Spectral features	Spectral entropy, wavelet decomposition	General-purpose features for comparison

fMRI Feature Recommendations:

Feature Category	Specific Features	Theoretical Basis
Region-of-interest	Amygdala, vmPFC, insula, orbitofrontal cortex activation	Low-fear model, IES account
Functional connectivity	Amygdala-vmPFC connectivity, fronto-limbic connectivity	Disrupted emotion regulation circuitry
Network-level	Default mode network, salience network integrity	Broader network dysfunction
Texture descriptors	GLCM features from activation maps	General-purpose image features

Feature sets should include the theory-motivated features from Layer 1 (frontal theta/beta ratio, spectral entropy, region-of-interest activation and connectivity in amygdala/vmPFC/insula circuits) alongside general-purpose features (power spectral density, wavelet decomposition, texture descriptors such as GLCM for image-derived maps) so the theory-driven features can be evaluated for incremental predictive value over generic ones.

Model selection should be sample-size-aware. Deep architectures such as CNNs (fMRI) and LSTM or transformer variants (EEG time series) are appropriate only where sample sizes are large enough to support them; in the small-to-moderate sample

regimes typical of forensic neuroimaging cohorts (often tens to low hundreds of participants), classical models with engineered features, such as support vector machines, random forests, or regularized regression, frequently outperform deep networks and should be treated as a required baseline, not a discarded alternative. Where deep learning is used, transfer learning from larger adjacent-domain datasets and strong regularization are advisable.

Multimodal fusion should occur at an intermediate representational level. Intermediate-level attention-based multimodal fusion, in which EEG- and fMRI-derived representations are combined at a shared representational layer rather than at the raw input or final-decision level, is the fusion strategy most consistently associated with both accuracy gains and interpretability gains in the adjacent literature reviewed in Section 2, and is the approach we recommend as the framework's default.

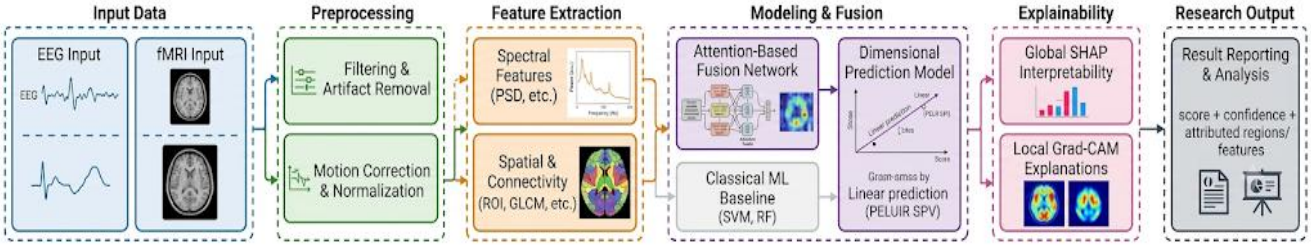

FIGURE 2: Proposed end-to-end pipeline

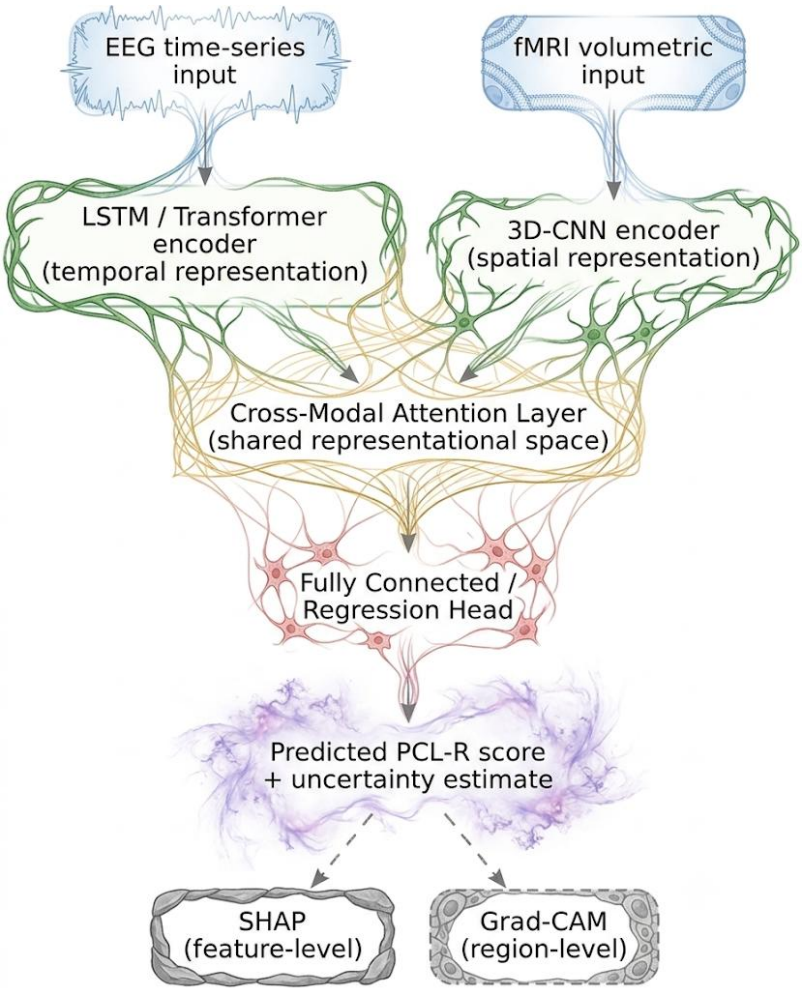

FIGURE 3: Internal architecture of attention-based fusion module

3.4 Layer 4: Validation and Translational Layer

This is the layer most often skipped in early-stage proposals, and the one reviewers scrutinize most closely. We recommend three concrete requirements:

1) **Cross-cohort or cross-site validation:** Train on one available cohort and test on an independent one, even if this means smaller effective sample sizes, since within-cohort cross-validation alone has been repeatedly shown to overstate real-world generalization in psychiatric neuroimaging classification [8].
2) **Explainability tied back to theory:** SHAP or Grad-CAM-style attributions should be checked against the Layer 1 theoretical prediction (e.g., do high-attribution regions correspond to amygdala/vmPFC or frontal theta features), and discrepancies should be reported and discussed rather than omitted. Negative or discrepant explainability findings are scientifically informative and should not be suppressed.
3) **Explicit statement of intended use:** Any resulting model should be framed as a research or hypothesis-generation tool and not as a diagnostic or forensic risk-assessment instrument, a distinction elaborated in Section 5.

TABLE 1
FOUR-LAYER CONCEPTUAL FRAMEWORK FOR AI-BASED PSYCHOPATHY-RELATED NEUROIMAGING RESEARCH

Layer	Core Question	Minimum Requirement
1. Theoretical	What neurocognitive account motivates the chosen features?	Explicit citation to a theory (e.g., low-fear model, IES) linked to each feature category
2. Data/Labeling	What is being predicted, and from whom?	Continuous PCL-R/PPI-R score or clearly-flagged proxy construct; documented cohort type; consideration of factor structure
3. Computational	What model is appropriate given sample size and modality?	Classical-ML baseline reported alongside any deep model; fusion at intermediate representational layer
4. Validation	Does the model generalize, and is it explainable?	Cross-cohort test; explainability output checked against Layer 1 theory; stated non-diagnostic intended use

IV. RESEARCH AGENDA: WHAT WORK REMAINS TO BE DONE

This section is written for researchers deciding where to direct empirical effort. Items are grouped by the framework layer they primarily address and roughly ordered by tractability.

4.1 Data Infrastructure

1) **Establish or extend consortia-style data-sharing agreements** among forensic and clinical sites that already collect PCL-R scores alongside EEG or fMRI, modeled on how multi-site consortia accelerated schizophrenia and Alzheimer's neuroimaging research. Given the sensitivity of forensic data, restricted-access data models with appropriate governance should be prioritized.
2) **Publish harmonized preprocessing pipelines and minimum reporting standards** specific to psychopathy-relevant cohorts, addressing the heterogeneity problem documented in adjacent EEG classification reviews.
3) **Where PCL-R-scored neuroimaging data cannot be obtained**, systematically validate proxy-construct datasets (callous-unemotional traits, antisocial personality measures) against small PCL-R-scored calibration samples to quantify how well proxy findings transfer.

4.2 Modeling

1) **Benchmark classical ML baselines against deep architectures** on the same cohort and splits, since current literature suggests classical models are competitive or superior at typical forensic-cohort sample sizes.
2) **Develop and evaluate intermediate-fusion, attention-based EEG-fMRI architectures** specifically for dimensional (regression/ordinal) psychopathy-score prediction, rather than adapting binary-classification architectures from other disorders.
3) **Test whether theory-motivated features** (frontal theta/beta ratio; amygdala-vmPFC connectivity) provide incremental predictive value over generic spectral/textural features, directly testing the theoretical layer rather than assuming it.

4) **Evaluate factor-specific modeling:** Determine whether predicting Factor 1 and Factor 2 scores separately yields more informative or generalizable results than predicting total PCL-R score.

4.3 Validation and Reporting

1) **Adopt pre-registration of hypotheses, feature sets, and validation splits** before model training, addressing the information-leakage and inflated-accuracy concerns raised in prior systematic reviews of psychiatric neuroimaging classification.
2) **Report performance with confidence intervals and cross-cohort replication,** not single-split accuracy figures.
3) **Report explainability outputs even when they contradict the motivating theory;** negative or discrepant explainability findings are scientifically informative and should not be omitted.

4.4 Translational and Policy Research

1) **Engage forensic psychology and legal scholars early** to define what, if any, appropriate downstream use cases exist, and to pre-empt the significant risk of misuse in high-stakes legal contexts such as sentencing or parole determinations.
2) **Study clinician and stakeholder trust and interpretability requirements** directly, following the template of explainability-and-trust studies conducted in other diagnostic-imaging domains, before any deployment discussion is appropriate.

V. ETHICAL CONSIDERATIONS

Work in this area carries elevated risk relative to most psychiatric-neuroimaging AI research, for reasons specific to the construct rather than the method.

- **Labeling risk:** An automated system that outputs a psychopathy-related score or classification could be misused to label individuals in legal, employment, or custodial contexts far beyond what the underlying evidence supports. Any model built under this framework should be explicitly scoped as a research tool for hypothesis generation, not a diagnostic or forensic risk-assessment instrument, and this scope limitation should be stated in any resulting publication, not left implicit.
- **Construct and measurement uncertainty:** Because PCL-R itself has documented cross-population and cross-rater variability, an AI model trained on PCL-R labels inherits that measurement uncertainty and should never be presented as more objective or more accurate than the label it was trained on. The distinction between Factor 1 and Factor 2 further complicates interpretation, and any model should report results separately for each factor where possible.
- **Data privacy and consent:** Neuroimaging data from forensic or clinical populations, particularly incarcerated populations, requires heightened consent and data-governance standards given the potential for coercion and the sensitivity of both the neuroimaging and the psychopathy-assessment data involved. Restricted-access data models should be preferred over open-access models where participant confidentiality cannot be adequately protected.
- **Stigma:** Psychopathy, more than most constructs addressed by psychiatric-neuroimaging AI, is subject to public and media narratives that could amplify stigma or determinism (e.g., 'criminal brain' framing) if findings are reported without appropriate uncertainty and scope caveats.
- **Cultural and demographic considerations:** PCL-R norms and correlates may differ across cultural and demographic groups. AI models trained on one population may perpetuate or amplify these differences if deployed uncritically. Researchers should document the demographic composition of training samples and explicitly state the limits of generalizability.
- **Error asymmetries:** In a forensic context, false positives could lead to unjustified restriction of liberty; false negatives could lead to inadequate supervision. These different error types have different ethical weights and should be discussed explicitly in any research reporting.
- **Algorithmic fairness:** Consideration should be given to whether AI models trained on predominantly male forensic samples would generalize to female or non-forensic populations, and how this should be addressed in model development and reporting.

These considerations should inform not only downstream deployment decisions but the research design itself; for example, they motivate the dimensional-scoring and cross-cohort-validation requirements set out in Section 3, since a poorly validated binary classifier is precisely the artifact most likely to be misused.

VI. DISCUSSION

The framework proposed here departs from a common pattern in early-stage proposals in this space, which typically pair an ambitious multimodal deep-learning architecture with an assumed high accuracy target (commonly stated as being above 85 percent) before a suitable labeled dataset has been identified or a theoretical rationale established for the chosen features. We have argued that this ordering should be reversed: theory and data strategy should constrain model choice, not the other way around, and reported performance should be earned through cross-cohort validation rather than asserted as a target.

The absence of a large, open, PCL-R-labeled EEG/fMRI dataset is the single largest obstacle to progress in this area, and no modeling innovation can substitute for it. We therefore view data infrastructure and multi-site collaboration, not novel architectures, as the highest-priority item on the research agenda in Section 4. Where deep multimodal architectures are appropriate, the literature reviewed in Section 2 suggests that intermediate, attention-based fusion combined with theory-anchored explainability offers the best available template, but this remains an empirical question specific to psychopathy-relevant data that has not yet been tested at scale.

A further consideration is what constitutes "success" in this domain. Unlike binary classification tasks where accuracy above a threshold is meaningful, a dimensional prediction task should be evaluated by metrics such as explained variance (R^2), correlation between predicted and actual scores, or calibration of predictions across the score range. Researchers should define success criteria before model training and report performance transparently, including cases where models fail to outperform simple baselines.

The role of Factor 1 versus Factor 2 in neuroimaging models deserves particular attention. Given the differential neural correlates of these factors, a model that predicts total PCL-R score may obscure meaningful dissociations. We recommend that future empirical work report results for Factor 1 and Factor 2 separately, even if the primary target is total score, to enable meta-analytic synthesis across studies.

Finally, we note that even a well-validated dimensional model of PCL-R correlates would not establish that the identified neuroimaging features are causally related to psychopathic traits, nor that they are specific to psychopathy rather than shared with other externalizing or personality disorders. These limitations should be acknowledged explicitly in any empirical report building on this framework.

VII. CONCLUSION

We have proposed a four-layer conceptual framework—theoretical grounding, data and labeling strategy, computational modeling, and validation—intended to guide future AI-based research into EEG and neuroimaging correlates of psychopathic traits. Rather than presenting a trained classifier and associated performance figures, we have argued that the field's most valuable near-term contribution is methodological discipline: dimensional rather than binary labeling, theory-anchored rather than arbitrary feature selection, classical-model baselines alongside deep architectures, cross-cohort rather than within-cohort validation, and an explicit, non-diagnostic statement of intended use. We have also emphasized the importance of distinguishing between PCL-R Factor 1 and Factor 2 in modeling and interpretation, and of addressing the specific ethical challenges that distinguish psychopathy research from other psychiatric-neuroimaging AI applications.

We hope this framework is useful to research groups with access to appropriate forensic or clinical cohorts, and we highlight data infrastructure and multi-site collaboration as the highest-priority unmet need in this area. By adopting the principles outlined here, the field can move beyond proof-of-concept studies and toward reproducible, generalizable, and ethically defensible research on the neurocognitive correlates of psychopathic traits.

CONFLICT OF INTEREST

The authors declare no conflict of interest.

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