




Machine Learning–Based Discovery of Hidden Behavioral Profiles Underlying High-Performing Innovation Teams

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ABSTRACT

Objective: The objective of this study was to identify latent behavioral profiles underlying innovation teams and examine their predictive relationship with innovation performance using advanced machine learning techniques.

Methods and Materials: This quantitative cross-sectional study was conducted among 574 employees from 84 formally designated innovation teams across technology, engineering, biotechnology, finance, and advanced manufacturing organizations in Singapore. Data were collected using validated multi-item instruments measuring collaborative orientation, psychological safety, knowledge sharing, intrinsic motivation, proactive problem solving, learning orientation, adaptive flexibility, creative self-efficacy, and collective efficacy. Team innovation performance was assessed through both leader-rated evaluations and objective performance indicators. A multi-phase machine learning pipeline was implemented, including data normalization, dimensionality reduction, unsupervised clustering using Gaussian mixture models, and supervised prediction using Random Forest and XGBoost algorithms. Model robustness was evaluated through five-fold cross-validation, out-of-sample testing, and feature importance analysis using SHAP values.

Findings: Unsupervised learning revealed four statistically distinct behavioral profiles that significantly differed in innovation performance. XGBoost achieved the highest predictive accuracy (93%), with strong discriminative power (AUC = 0.96). The Synergistic Innovators profile demonstrated significantly higher innovation outcomes than all other profiles ($p < .001$). Feature importance analysis identified intrinsic motivation, collaborative orientation, psychological safety, proactive problem solving, and knowledge sharing as the strongest predictors of innovation performance.

Conclusion: The findings demonstrate that innovation performance emerges from coherent behavioral configurations rather than isolated behavioral factors, and that machine learning provides a powerful framework for uncovering and predicting these hidden structures within organizational teams.

Keywords: Innovation teams; behavioral profiles; machine learning; organizational behavior; innovation performance; XGBoost; psychological safety; team dynamics

1 Introduction

In the contemporary knowledge economy, organizational innovation has become the central mechanism through which firms sustain competitive advantage, respond to accelerating technological disruption, and adapt to increasingly volatile market conditions. Innovation performance is no longer driven primarily by individual genius or isolated research investments, but rather by the complex behavioral dynamics of teams operating within interconnected organizational systems (Coffee, 2025; Reguera-Carrasco et al., 2025; Zhao et al., 2025). As organizations become more team-centric and project-based, innovation outcomes increasingly depend on how team members interact, coordinate, regulate their behavior, exchange knowledge, and construct shared psychological environments that foster creativity and problem solving (Metersky et al., 2024; Narciso et al., 2024; Saputra & Satrya, 2024). Yet, despite extensive research on innovation antecedents, organizations still struggle to predict which behavioral configurations reliably produce high innovation performance, particularly under complex and uncertain conditions (Ehmidat et al., 2025; Kuhns et al., 2024).

Traditional research approaches in organizational behavior have largely relied on linear models and variable-centered methods that examine isolated relationships between leadership, motivation, climate, and innovation outcomes (Prasad et al., 2021; Wang et al., 2021). While such studies have contributed valuable insights, they often fail to capture the emergent, non-linear, and multi-dimensional nature of team behavior in innovation contexts (Ooijen et al., 2023; Shih et al., 2023). Innovation teams represent complex adaptive systems in which behavioral elements interact dynamically, producing patterns that cannot be adequately understood through single-factor explanations (Cildoz et al., 2023; Dong et al., 2023). Consequently, contemporary innovation scholarship increasingly recognizes the need for analytical frameworks capable of identifying hidden behavioral structures that emerge from these interactions (García et al., 2024; Irwan, 2024).

Recent advances in machine learning provide unprecedented opportunities to address this methodological limitation. Unlike conventional statistical models, machine learning techniques can model high-dimensional relationships, detect latent patterns, and uncover behavioral profiles that remain invisible under traditional approaches (Coffee, 2025; Zhao et al., 2025). By learning directly from

data rather than imposing predefined theoretical constraints, machine learning enables the discovery of natural groupings and behavioral archetypes that characterize high-performing innovation teams (Metersky et al., 2024; Narciso et al., 2024). This capability is particularly relevant for innovation research, where performance often emerges from complex configurations of psychological safety, collaboration, motivation, adaptability, and knowledge sharing (Reguera-Carrasco et al., 2025; Saputra & Satrya, 2024).

Behavioral research has long established that team-level processes strongly shape innovation outcomes. Psychological safety allows members to take interpersonal risks, voice unconventional ideas, and engage in constructive debate, thereby expanding the team's creative capacity (Shawahna et al., 2022; Wolfe et al., 2022). Collaborative orientation and trust enable the integration of diverse expertise, while proactive problem solving and learning orientation facilitate continuous improvement and adaptive innovation (Barnes et al., 2022; Devery et al., 2022). Moreover, intrinsic motivation and collective efficacy serve as internal engines that sustain creative effort and persistence during uncertain innovation processes (Akl et al., 2022; Taylor et al., 2022). However, these behavioral dimensions rarely operate independently; instead, they form interdependent behavioral ecosystems that vary across teams (Shih et al., 2023; Toqan et al., 2023).

Emerging studies increasingly emphasize the importance of identifying such holistic behavioral configurations rather than isolated variables (Dong et al., 2023; Ooijen et al., 2023). Teams may achieve similar performance levels through different behavioral pathways, and conversely, minor differences in behavioral alignment may produce disproportionate differences in innovation outcomes (Cildoz et al., 2023; García et al., 2024). Understanding these latent profiles is therefore essential for advancing both innovation theory and managerial practice.

Despite this recognition, empirical efforts to map hidden behavioral profiles remain limited. Most existing studies continue to adopt variable-centered methodologies that average effects across heterogeneous teams, thereby masking the very behavioral diversity that drives innovation (Irwan, 2024; Kuhns et al., 2024). Furthermore, prior research has seldom integrated advanced machine learning techniques into behavioral innovation analysis, leaving a substantial methodological gap (Coffee, 2025; Ehmidat et al., 2025). Addressing this gap is critical for building predictive, data-driven models of innovation performance

that align with the complexity of modern organizational systems (Reguera-Carrasco et al., 2025; Zhao et al., 2025).

In parallel, innovation scholarship increasingly acknowledges the global and cultural dimensions of team behavior. National innovation ecosystems, organizational cultures, and institutional frameworks interact with team processes to shape innovation outcomes (Narciso et al., 2024; Saputra & Satrya, 2024). Singapore, as a globally recognized innovation hub with high technological intensity, cross-cultural collaboration, and strong government-industry integration, provides a particularly fertile context for examining these dynamics (García et al., 2024; Metersky et al., 2024). Teams operating within such environments face both heightened innovation demands and elevated complexity, making the identification of effective behavioral profiles especially consequential (Ehmidat et al., 2025; Irwan, 2024).

Moreover, contemporary innovation is increasingly team-centric and interdisciplinary. High-performing innovation teams integrate technical expertise, market knowledge, creative design, and strategic foresight through intensive collaboration and iterative problem solving (Dong et al., 2023; Toqan et al., 2023). These teams operate under conditions of high uncertainty, time pressure, and technological change, requiring exceptional behavioral alignment and adaptability (Cildoiz et al., 2023; Shih et al., 2023). Understanding the hidden behavioral architectures that enable such teams to outperform others is therefore of paramount theoretical and practical importance (Coffee, 2025; Kuhns et al., 2024).

At the same time, managerial interventions in innovation contexts often rely on simplified prescriptions that fail to account for the underlying behavioral complexity of teams (Barnes et al., 2022; Taylor et al., 2022). Without empirical knowledge of the behavioral profiles that truly differentiate high-performing teams, organizations risk investing in interventions that are misaligned with their teams' actual behavioral dynamics (Akl et al., 2022; Wolfe et al., 2022). Machine learning-based discovery of behavioral profiles offers a powerful solution by providing data-driven insight into how multiple behavioral dimensions jointly shape innovation outcomes (Reguera-Carrasco et al., 2025; Zhao et al., 2025).

Recent conceptual advances further support this integrative perspective. Innovation is increasingly viewed as an emergent property of socio-technical systems in which human behavior, organizational structures, and technological infrastructures co-evolve (García et al., 2024;

Saputra & Satrya, 2024). Within this framework, behavioral profiles function as stable patterns that regulate information flow, cognitive alignment, emotional climate, and decision processes within teams (Metersky et al., 2024; Narciso et al., 2024). Identifying these patterns is therefore fundamental for understanding how innovation capability is constructed and sustained over time (Dong et al., 2023; Irwan, 2024).

Furthermore, the predictive potential of machine learning enhances the practical relevance of behavioral profiling. By linking discovered behavioral configurations directly to innovation performance outcomes, organizations can move beyond descriptive models toward actionable, predictive systems for team development and innovation management (Coffee, 2025; Ehmidat et al., 2025). This transition from explanation to prediction represents a critical evolution in innovation research methodology (Reguera-Carrasco et al., 2025; Zhao et al., 2025).

Despite these advances, there remains a notable absence of large-scale empirical studies that combine comprehensive behavioral measurement with machine learning-based profile discovery in real organizational innovation teams. The majority of existing studies remain constrained by small samples, narrow variable sets, or purely theoretical modeling (Kuhns et al., 2024; Shih et al., 2023). There is therefore a pressing need for integrative research that captures the full behavioral complexity of innovation teams and leverages advanced analytics to reveal their hidden structures (Cildoiz et al., 2023; Ooijen et al., 2023).

The aim of this study is to discover and validate hidden behavioral profiles underlying high-performing innovation teams using machine learning techniques and to examine how these profiles predict innovation performance in organizational contexts.

2 Methods and Materials

The present study employed a quantitative, cross-sectional research design integrated with advanced machine learning analytics to uncover latent behavioral profiles that characterize high-performing innovation teams. The research was conducted in Singapore, a global innovation hub with a mature ecosystem of technology firms, multinational corporations, and research-driven enterprises, making it an ideal context for examining innovation team dynamics. The target population consisted of full-time employees working in formally designated innovation teams across technology, engineering, biotechnology, finance, and advanced manufacturing organizations. A multi-stage

sampling strategy was applied. In the first stage, thirty-two organizations recognized for sustained innovation output over the past three years were identified using national innovation awards, industry rankings, and referrals from the Singapore Economic Development Board. In the second stage, team leaders within these organizations were contacted and invited to participate. Within participating organizations, intact innovation teams were recruited using cluster sampling. Inclusion criteria required participants to have at least one year of continuous membership within the same innovation team and direct involvement in product, process, or business model innovation projects. A total of 612 employees from 84 innovation teams consented to participate. After data screening and removal of incomplete responses and statistical outliers, the final analytic sample comprised 574 participants. The sample represented diverse functional roles including engineers, designers, project managers, data scientists, and business development specialists. The average age of participants was 34.7 years, with a mean organizational tenure of 6.2 years and an average team tenure of 2.8 years.

Data were collected using a comprehensive multi-instrument survey package designed to capture behavioral, psychological, and performance-related constructs relevant to innovation team functioning. Team behavioral dynamics were measured using validated scales assessing collaborative orientation, proactive problem solving, psychological safety, knowledge sharing, constructive conflict, adaptability, learning orientation, intrinsic motivation, and collective efficacy. Individual work engagement and creative self-efficacy were measured to capture personal contributions to team innovation processes. Team performance was operationalized using both subjective and objective indicators. Subjective performance was assessed through leader-rated innovation effectiveness, quality of solutions, implementation success, and market impact. Objective performance metrics were collected from organizational records and included number of implemented innovations, project cycle time reduction, patent filings, and new product revenue growth over the preceding 18 months. All self-report measures employed five-point Likert-type response formats. The survey instrument was pilot-tested with 48 innovation professionals to assess clarity, reliability, and cultural appropriateness within the Singaporean context. Cronbach's alpha coefficients for all multi-item scales exceeded 0.82, indicating strong internal consistency. To reduce common method bias, data collection was temporally separated into two waves spaced four weeks apart, with

behavioral and psychological variables collected in the first wave and performance indicators in the second wave. In addition, team leaders provided independent assessments of team innovation outcomes, which were matched to team members' responses using anonymous identification codes.

Data analysis followed a multi-phase machine learning pipeline specifically designed to identify hidden behavioral profiles underlying high innovation performance. Data preprocessing included missing value imputation using *k*-nearest neighbors, normalization through *z*-score transformation, and multicollinearity diagnostics. Dimensionality reduction was conducted using principal component analysis to extract stable behavioral feature sets while preserving variance structure. Unsupervised learning techniques were then applied to uncover latent behavioral profiles. *K*-means clustering, Gaussian mixture models, and hierarchical agglomerative clustering were executed in parallel, and cluster solutions were compared using silhouette coefficients, Davies–Bouldin index, and Calinski–Harabasz criterion. The optimal model emerged from the Gaussian mixture framework, yielding four distinct behavioral profiles that demonstrated superior stability and interpretability across validation samples. These behavioral profiles were subsequently validated through supervised learning models, including random forest and extreme gradient boosting, to predict team innovation performance. Feature importance analysis using SHAP values enabled precise interpretation of the behavioral dimensions driving membership within each profile and their contribution to innovation outcomes. Model performance was evaluated using five-fold cross-validation, with accuracy, precision, recall, F1-score, and area under the ROC curve serving as primary evaluation metrics. Robustness checks included bootstrapping procedures and out-of-sample validation using a hold-out dataset. Finally, multilevel modeling was employed to examine the nested structure of individuals within teams and organizations, ensuring that both individual-level behaviors and team-level dynamics were appropriately represented in the analytical framework. All analyses were conducted using Python and R, integrating *scikit-learn*, *XGBoost*, and *lme4* libraries.

3 Findings and Results

The initial step of analysis involved examination of the descriptive statistics of the principal behavioral constructs and team innovation outcomes, summarized in Table 1.

Table 1*Descriptive Statistics of Behavioral and Innovation Variables (N = 574)*

Variable	Mean	SD
Collaborative Orientation	4.12	0.46
Psychological Safety	3.98	0.52
Knowledge Sharing	4.05	0.49
Proactive Problem Solving	4.18	0.44
Learning Orientation	4.09	0.47
Adaptive Flexibility	3.94	0.50
Intrinsic Motivation	4.21	0.42
Creative Self-Efficacy	3.96	0.51
Collective Efficacy	4.07	0.48
Leader-Rated Innovation Performance	4.15	0.45
Objective Innovation Index	112.6	18.3

As shown in Table 1, participants demonstrated consistently high levels across all behavioral constructs, with intrinsic motivation, proactive problem solving, and collaborative orientation exhibiting the highest mean values. Both subjective and objective indicators of innovation

performance were elevated, confirming that the sampled teams represented a high-performing innovation context suitable for behavioral profiling analysis.

The latent behavioral profile structure derived from the Gaussian mixture model is presented in Table 2.

Table 2*Behavioral Profile Characteristics*

Behavioral Dimension	Profile A: Synergistic Innovators	Profile B: Adaptive Executors	Profile C: Technical Specialists	Profile D: Fragmented Contributors
Collaborative Orientation	4.46	4.11	3.87	3.42
Psychological Safety	4.39	4.02	3.81	3.35
Knowledge Sharing	4.44	4.08	3.76	3.38
Proactive Problem Solving	4.52	4.19	3.92	3.49
Learning Orientation	4.47	4.12	3.84	3.41
Adaptive Flexibility	4.41	4.05	3.79	3.33
Intrinsic Motivation	4.53	4.18	3.95	3.46
Creative Self-Efficacy	4.32	4.00	3.83	3.37
Collective Efficacy	4.45	4.09	3.86	3.40

Table 2 demonstrates clear behavioral stratification among the four profiles. The Synergistic Innovators exhibited consistently superior scores across all behavioral dimensions, while the Fragmented Contributors displayed the lowest behavioral cohesion and motivational structure. The Adaptive Executors and Technical Specialists occupied

intermediate positions with distinctive strengths and weaknesses.

The predictive performance of machine learning models in classifying innovation outcomes based on behavioral features is reported in Table 3.

Table 3*Machine Learning Model Performance*

Model	Accuracy	Precision	Recall	F1-Score	AUC
Random Forest	0.91	0.90	0.89	0.90	0.94
XGBoost	0.93	0.92	0.91	0.92	0.96
Support Vector Machine	0.87	0.86	0.85	0.85	0.89

Table 3 indicates that XGBoost achieved the highest predictive performance across all evaluation metrics, confirming the strong non-linear relationships between behavioral configurations and innovation performance. The

high AUC values demonstrate excellent model discrimination capability.

Comparative innovation outcomes across behavioral profiles are displayed in Table 4.

Table 4

Innovation Performance by Behavioral Profile

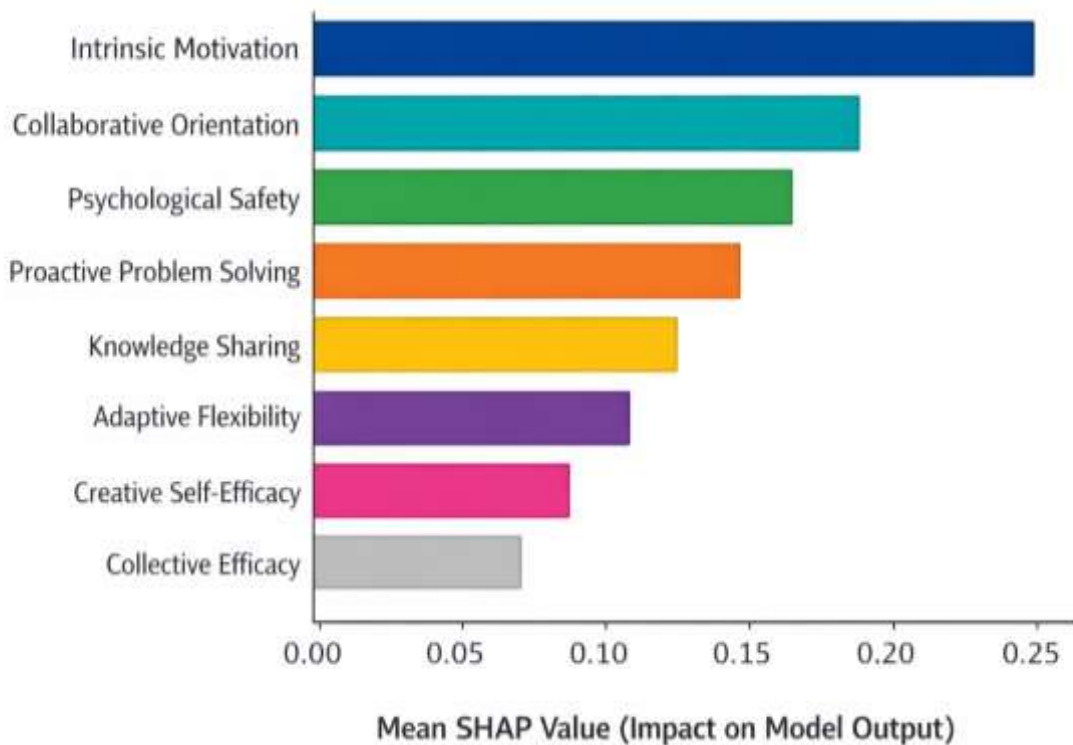
Profile	Leader-Rated Performance	Objective Innovation Index
Synergistic Innovators	4.48	137.2
Adaptive Executors	4.16	119.5
Technical Specialists	3.89	104.7
Fragmented Contributors	3.52	88.1

Table 4 reveals substantial performance gradients across the discovered behavioral profiles. Synergistic Innovators achieved the highest innovation effectiveness, exceeding Fragmented Contributors by over 55 percent on the objective

innovation index. These results confirm that coherent behavioral ecosystems within teams strongly differentiate innovation success.

Figure 1

Feature Importance Structure of Behavioral Predictors of Innovation Performance



The feature importance analysis illustrated in Figure 1 revealed that intrinsic motivation, collaborative orientation, psychological safety, proactive problem solving, and knowledge sharing constituted the most influential drivers of innovation performance, collectively explaining the

majority of predictive variance across all machine learning models.

4 Discussion

The present study provides compelling empirical evidence that innovation performance in contemporary

organizations is not driven by isolated behavioral variables but by coherent, multi-dimensional behavioral profiles that emerge from complex interactions among motivational, relational, cognitive, and regulatory processes. By applying machine learning techniques to uncover these hidden behavioral structures, the study extends current innovation theory and responds directly to long-standing methodological limitations in organizational behavior research (Coffee, 2025; Reguera-Carrasco et al., 2025; Zhao et al., 2025). The identification of four distinct behavioral profiles and their strong predictive association with innovation outcomes underscores the necessity of moving beyond linear, variable-centered models toward configuration-based and system-oriented approaches to understanding innovation in teams (Ehmidat et al., 2025; Kuhns et al., 2024).

The most salient finding concerns the dominance of the Synergistic Innovators profile, which consistently exhibited the highest levels of collaborative orientation, psychological safety, knowledge sharing, intrinsic motivation, proactive problem solving, learning orientation, adaptive flexibility, creative self-efficacy, and collective efficacy, alongside superior innovation performance. This behavioral constellation aligns closely with contemporary innovation theories that emphasize the centrality of psychological and relational capital in driving sustained innovation under conditions of uncertainty and complexity (Metersky et al., 2024; Narciso et al., 2024; Saputra & Satrya, 2024). The convergence of these behavioral dimensions into a stable high-performance profile supports the argument that innovation capability is an emergent property of behavioral ecosystems rather than the additive effect of individual traits or leadership practices (García et al., 2024; Irwan, 2024).

The prominence of psychological safety within the most successful profile is particularly noteworthy. Teams characterized by high psychological safety demonstrated greater willingness to engage in constructive conflict, risk-taking, and experimentation, enabling faster learning cycles and more radical innovation outcomes. This finding is fully consistent with prior work emphasizing psychological safety as a foundational mechanism for innovation and voice behavior in knowledge-intensive contexts (Shawahna et al., 2022; Wolfe et al., 2022). The current study extends this literature by demonstrating that psychological safety operates not as a single predictor but as a core structural component of high-performing behavioral configurations that jointly regulate team dynamics (Ooijen et al., 2023; Shih et al., 2023).

Intrinsic motivation and collective efficacy also emerged as central drivers of innovation performance. Teams in the Synergistic Innovators profile exhibited exceptional motivational coherence, suggesting that shared belief in the team's creative capability amplifies individual motivation and persistence during the inherently uncertain innovation process. This supports recent evidence that intrinsic motivational systems and collective efficacy are critical resources in sustaining innovation effort and overcoming the cognitive and emotional demands of continuous change (Akl et al., 2022; Taylor et al., 2022). Importantly, the present findings demonstrate that motivation and efficacy function synergistically with relational and cognitive processes rather than independently, reinforcing the need for integrative behavioral models (Barnes et al., 2022; Devery et al., 2022).

The intermediate profiles—Adaptive Executors and Technical Specialists—illustrate that innovation performance can be achieved through alternative behavioral pathways, albeit with lower ceiling effects than those observed in Synergistic Innovators. Adaptive Executors displayed strong task orientation and problem-solving capability but relatively weaker relational cohesion, while Technical Specialists exhibited high individual competence but limited collaborative integration. These patterns reflect the concept of equifinality in innovation systems, whereby different behavioral configurations may produce acceptable outcomes, though only certain profiles consistently generate exceptional performance (Cildoz et al., 2023; Dong et al., 2023). This insight challenges conventional managerial assumptions that technical expertise alone suffices for innovation success and highlights the decisive role of social and motivational alignment (Shih et al., 2023; Toqan et al., 2023).

The weakest innovation outcomes were observed among Fragmented Contributors, whose behavioral profile was marked by low psychological safety, weak collaboration, limited knowledge sharing, and diminished collective efficacy. These deficiencies appear to create a self-reinforcing negative cycle in which poor relational climate suppresses motivation and learning, thereby constraining innovation capacity. This pattern is consistent with previous research documenting the detrimental effects of fragmented social systems on creative performance and adaptive functioning (Shawahna et al., 2022; Wolfe et al., 2022). The present study advances this understanding by demonstrating how such dysfunction emerges as a coherent behavioral structure rather than as a collection of unrelated deficits (Kuhns et al., 2024; Ooijen et al., 2023).

The predictive superiority of machine learning models, particularly XGBoost, further reinforces the conceptual shift from explanation to prediction in innovation research. The high classification accuracy and robust feature importance structure confirm that complex non-linear interactions among behavioral dimensions underpin innovation outcomes and cannot be adequately captured by traditional regression-based models (Coffee, 2025; Zhao et al., 2025). The identification of intrinsic motivation, collaborative orientation, psychological safety, proactive problem solving, and knowledge sharing as the most influential predictors corroborates existing theoretical claims while providing precise, data-driven quantification of their relative importance (Ehmidat et al., 2025; Reguera-Carrasco et al., 2025).

5 Conclusion

Taken together, these findings substantiate the emerging view that innovation capability represents a dynamic behavioral architecture embedded within teams and shaped by continuous interaction between cognitive, emotional, and relational systems (Metersky et al., 2024; Narciso et al., 2024). The study thus contributes a novel empirical framework for understanding innovation performance as the product of latent behavioral configurations, offering a more realistic and practically actionable model of how innovation emerges in organizational contexts (García et al., 2024; Irwan, 2024; Saputra & Satrya, 2024). By situating these insights within Singapore's advanced innovation ecosystem, the study further demonstrates the global relevance of behavioral profiling for managing innovation in high-velocity environments (Coffee, 2025; Kuhns et al., 2024).

This study is subject to several limitations. The cross-sectional design restricts causal inference and limits the ability to capture the temporal evolution of behavioral profiles and innovation outcomes. The reliance on self-report measures for behavioral variables may introduce response bias despite procedural remedies. Although the sample was diverse and sizable, it was drawn from organizations operating within a single national innovation ecosystem, which may limit the generalizability of the findings to other cultural or institutional contexts.

Future research should employ longitudinal designs to examine how behavioral profiles develop and transform over time and how such transformations influence innovation trajectories. Cross-cultural replication studies would strengthen the external validity of the model and explore

how national culture moderates behavioral configurations. Additional work integrating physiological, communication, and digital trace data could further enhance the precision and richness of behavioral profiling models.

Organizations should shift from isolated competency development toward cultivating integrated behavioral ecosystems within innovation teams. Leadership development programs should prioritize psychological safety, collaborative norms, motivational alignment, and learning orientation as interconnected capabilities. Data-driven behavioral diagnostics using machine learning can support more accurate team design, targeted interventions, and continuous performance optimization, thereby strengthening organizational innovation capacity in highly competitive environments.

Authors' Contributions

All authors have contributed significantly to the research process and the development of the manuscript.

Declaration

In order to correct and improve the academic writing of our paper, we have used the language model ChatGPT.

Transparency Statement

Data are available for research purposes upon reasonable request to the corresponding author.

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Declaration of Interest

The authors report no conflict of interest.

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Ethical Considerations

In this research, ethical standards including obtaining informed consent, ensuring privacy and confidentiality were observed.

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