Ontology-Based Graph Transformer Network for Robust Bearing Fault Diagnosis under Unseen Operating Conditions

Yong Hun Park[1], Seo Won Lee[1], Chan Hee Park[2] and Joon Ha Jung[1,*]

[1]*Department of Industrial Engineering, Ajou University, Suwon, Gyeonggi-do, 16499, Republic of Korea*

[2]*Department of Mechanical and Information Engineering, University of Seoul, Seoul, 02504, Republic of Korea*

dydtm1225@ajou.ac.kr
seowon@ajou.ac.kr
chnypark@uos.ac.kr
joonha@ajou.ac.kr

ABSTRACT

Conventional data-driven diagnostic models for rotating machinery often exhibit limited generalization under varying operating conditions. Signal-based approaches typically rely on condition-dependent training data and statistical feature learning, making them vulnerable to domain shifts and complex fault scenarios. In particular, frequency-domain features are commonly treated as unstructured statistical descriptors, without capturing the physical relationships among characteristic frequencies such as harmonic and sideband structures intrinsically linked to bearing fault mechanisms. Consequently, the learned representations tend to overfit to the training distribution, leading to pronounced performance degradation under unseen operating conditions. These limitations highlight the need for diagnostic frameworks that incorporate physically grounded relational structures to achieve robust generalization.

To address these challenges, this study proposes OFG-GTN (Ontology-based Frequency Graph–GTN), an ontology-based bearing fault diagnosis framework that integrates structured frequency representation and relational graph learning. Vibration signals are transformed into ontology-based frequency graphs by encoding physically defined characteristic frequencies, harmonic relations, and sideband dependencies derived from bearing fault mechanics. A GTN is employed to perform graph-level fault classification by capturing higher-order relational dependencies among frequency components. Experimental results demonstrate that OFG-GTN achieves robust and generalizable bearing fault diagnosis across diverse operating conditions, including those not encountered during training.

1. INTRODUCTION

Rotating machinery plays an indispensable role in modern industrial systems, and rolling element bearings are among the most failure-prone components within such systems. Accurate and timely identification of bearing faults is essential for preventing catastrophic failures, minimizing unplanned downtime, and enhancing operational safety. With the rapid advancement of deep learning, data-driven diagnostic models, including convolutional neural networks, have demonstrated remarkable classification accuracy by learning discriminative patterns directly from raw vibration signals (Zhang et al., 2018). Despite these achievements, a fundamental limitation persists: conventional deep learning models rely exclusively on data-driven feature learning without incorporating structured domain knowledge, rendering them highly susceptible to performance degradation under operating conditions not encountered during training (Zhao et al., 2024).

A predominant approach in deep learning-based fault diagnosis employs frequency-domain features as model inputs; however, these features are typically extracted as isolated spectral amplitude values, leaving the structured dependencies among fault-related frequencies — such as harmonic progressions and sideband modulations — unmodeled (Lei et al., 2013). In rolling element bearings, fault-related frequencies are analytically governed by bearing geometry and rotational speed, giving rise to harmonic and sideband structures that are intrinsically linked to underlying fault mechanisms. When such physically grounded relational structures are not incorporated into the model representation, the learned features become tightly coupled to the statistical regularities of the training distribution, resulting in pronounced generalization failure under unseen operating conditions (Han et al., 2021).

To address this limitation, this study proposes OFG-GTN, an ontology-based explainable diagnostic framework that reformulates frequency-domain representations into structured relational graphs. Physically defined characteristic frequencies derived from bearing fault mechanics, together with their harmonic and sideband dependencies, are explicitly encoded into an ontology-based heterogeneous graph, wherein frequency components are represented as nodes and their physical dependencies as typed relational edges. Because this structured representation is grounded in the physical relationships governing bearing kinematics, which remain consistent across different operating conditions, it facilitates cross-domain generalization beyond the training distribution. A Graph Transformer Network (GTN) (Yun et al., 2019) is subsequently employed to capture higher-order relational dependencies among frequency components for graph-level fault classification.

The main contributions of this study are twofold: (1) we propose OFG-GTN that explicitly encodes harmonic progressions and sideband dependencies as typed relational edges, enabling structured fault-discriminative representations that remain invariant across varying operating conditions; and (2) we empirically demonstrate, for the first time, that physics-invariant relational representations grounded in bearing fault mechanics are robust to domain shift, enabling a GTN-based classifier to consistently outperform conventional data-driven and domain generalization baselines across all unseen operating conditions under a leave-one-out cross-domain evaluation.

The remainder of this paper is organized as follows. Section 2 formulates the bearing fault diagnosis problem and presents the theoretical background of Graph Transformer Networks. Section 3 describes OFG-GTN, encompassing ontology-based frequency graph construction and GTN-based fault classification. Section 4 presents experimental evaluations across unseen operating conditions to validate the generalization capability of OFG-GTN. Finally, Section 5 concludes the study and discusses limitations and future research directions.

2. Theoretical Background

This section presents the theoretical foundations of OFG-GTN. The bearing fault diagnosis problem is first formulated within a graph-based learning paradigm, followed by an introduction to the fundamental principles of GTN that underpin relational learning over ontology-based frequency graphs.

2.1. Problem Definition

Let $x(t) \in \mathbb{R}$ denote a time-domain vibration signal acquired from a rotating machinery system, where t represents discrete time samples. The objective is to predict a fault label $y \in \{1,2,\dots,C\}$, where C denotes the number of fault categories, including normal and various fault types. To extract fault-relevant information, the time-domain signal is transformed into the frequency domain using the Fourier transform. The resulting spectrum is given by Eq. (1):

$$X(f) = \mathcal{F}\{x(t)\} \tag{1}$$

where f represents frequency and $\mathcal{F}(\cdot)$ denotes the Fourier transform operator. In rolling element bearings, characteristic fault frequencies are analytically determined based on bearing geometric parameters and rotational speed. These physically derived frequencies—including outer-race fault frequency (Ball Pass Frequency Outer Race, BPFO), inner-race fault frequency (Ball Pass Frequency Inner Race, BPFI), and rotational frequency (f_r) serve as reference components for identifying corresponding spectral peaks in the frequency domain. In addition, harmonics and sidebands around these characteristic frequencies are extracted to capture modulation patterns associated with specific fault mechanisms. The extracted characteristic frequency components and their relational structures form the basis for constructing an ontology-based frequency graph.

Rather than treating the spectrum as an unstructured feature vector, this study reformulates the diagnosis problem as a graph-level classification task. Let a graph be defined as $G = (V, E, R)$, where V denotes the set of frequency-related nodes, E represents physically defined relationships such as harmonic and sideband connections, and R denotes the set of relation types. Each node $v \in V$ is associated with a feature vector derived from spectral attributes. Based on the structured representation G, a mapping function is learned to predict the graph label y. Thus, the fault diagnosis problem is redefined as learning a mapping as defined in Eq. (2):

$$\Phi : G \rightarrow y \tag{2}$$

where $\Phi(\cdot)$ is a graph-based classifier trained in a supervised manner.

2.2. Graph Transformer Network (GTN)

GTN are specifically designed to learn node representations on heterogeneous graphs, which consist of multiple types of nodes and edges that encode diverse relational semantics. Unlike conventional graph neural networks that operate on fixed homogeneous graph structures, GTNs are capable of adaptively transforming heterogeneous graph inputs into task-optimized relational structures, making them particularly well-suited for domains where multiple relation types coexist and interact in complex ways. A heterogeneous graph can be formally defined as $G = (V, E, R)$. For each relation type $r \in R$, a relation-specific adjacency matrix A_r is defined to capture structural connectivity under that relation.

In such heterogeneous graphs, significant structural dependencies may extend beyond direct neighbors and emerge through higher-order relational paths, commonly referred to as meta-paths. A meta-path represents a composite relation formed by sequentially combining multiple relation types, and the choice of meta-paths can substantially influence the quality of learned node representations. Learning effective meta-path structures is therefore critical for capturing high-order relational patterns embedded in the graph. However, manually designing meta-paths is often task-dependent and requires substantial domain expertise, which limits the scalability and generalizability of meta-path-based approaches.

To address this limitation, GTNs automatically learn useful meta-path structures through differentiable combinations of relation-specific adjacency matrices, eliminating the need for hand-crafted relational templates. Instead of manually defining composite relations, GTNs construct meta-path adjacency matrices as weighted combinations of relation-specific adjacency products. For example, a two-step meta-path composite adjacency matrix can be expressed as in Eq. (3):

$$A_{meta} = \sum_{r_i, r_j \in R} \alpha_{ij} A_{r_i} A_{r_j} \tag{3}$$

where A_{r_i} and A_{r_j} are adjacency matrices corresponding to relation types r_i and r_j, and α_{ij} denotes learnable weights. Through this mechanism, GTN enables adaptive learning of composite relational structures that enhance representation capability for downstream classification tasks.

3. The OFG-GTN Framework

OFG-GTN is designed around two core principles: explicit encoding of physically defined frequency relationships as graph structure, and relational learning over that structure via a GTN. This design decouples fault-discriminative representation from operating condition-specific statistical patterns, enabling robust diagnostic performance across different operating conditions. The overall architecture is illustrated in Figure 1. The framework consists of two main modules: (1) an ontology-based graph construction module, which transforms vibration signals into physically grounded heterogeneous graph representations, and (2) a GTN-based fault classification module, which learns structured relationships among frequency components for graph-level fault classification.

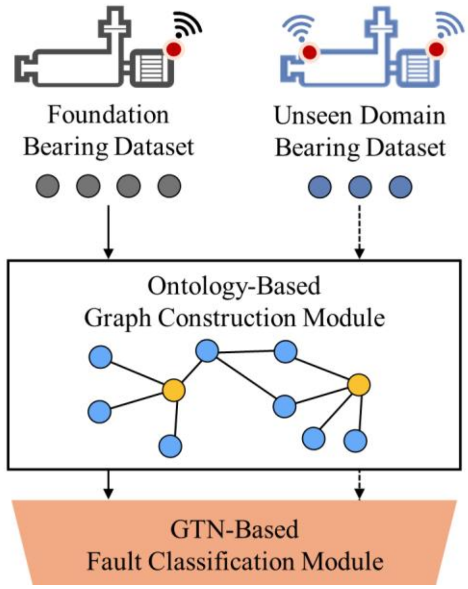


Figure 1. Overall framework of OFG-GTN.

3.1. Ontology-Based Graph Construction Module

To enable relational reasoning over physically meaningful frequency components, the graph construction module converts vibration signals into heterogeneous frequency graphs by mapping spectral observations onto a physically defined relational schema derived from bearing fault mechanics. This mapping ensures that each spectral peak is interpreted not as an isolated amplitude value, but as an element within a structured network of fault-related frequency dependencies.

First, the time-domain vibration signal $x(t)$ is transformed into the frequency domain via the Fourier transform. Based on the bearing geometric parameters and rotational speed, characteristic fault frequencies—namely BPFO, BPFI, and f_r —are analytically computed. These characteristic frequencies serve as physically defined reference components for identifying relevant spectral peaks. Spectral components that coincide with or lie within a predefined tolerance of these reference frequencies are detected and selected to form a set of candidate frequency components.

Next, the ontology-based frequency graph instantiates a heterogeneous structure $G = (V, E, R)$ with domain-specific node and relation definitions. The node set consists of two categories as shown in Eq. (4):

$$V = V_f \cup V_r \tag{4}$$

where V_f corresponds to frequency nodes and V_r corresponds to reference frequency nodes. Each frequency node $v \in V_f$ represents an observed spectral peak and is associated with a feature vector that encodes both signal-level evidence and physics-informed attributes. Specifically, the feature vector includes peak amplitude, harmonic order, sideband indicator, and the associated reference component (e.g., BPFO, BPFI, or f_r). Through this encoding, each peak is represented not merely as a numerical spectral component but as a structured element linked to a physically defined fault-related frequency.

The reference frequency nodes $v \in V_r$ are defined based on the analytically computed characteristic frequencies. Rather than representing raw numerical values alone, these nodes function as ontology anchors that explicitly encode the physical categories to which frequency nodes are related. In other words, reference nodes serve as semantic mediators that express which physically defined frequency component each observed peak corresponds to. This design structurally embeds domain knowledge into the graph by linking spectral evidence to fault-related physical concepts.

Edges are introduced to model structured relationships among frequency components. Two relation types are considered, as specified in Eq. (5).

$$R = \{harmonic, sideband\} \tag{5}$$

A harmonic relation is established when a peak frequency satisfies the condition defined in Eq. (6):

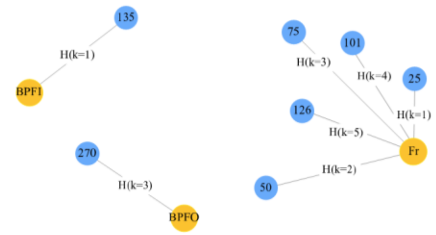
$$f_v = k f_c \tag{6}$$

where f_c denotes a reference frequency and k is a harmonic order integer within a predefined tolerance. A sideband relation is established as defined in Eq. (7):

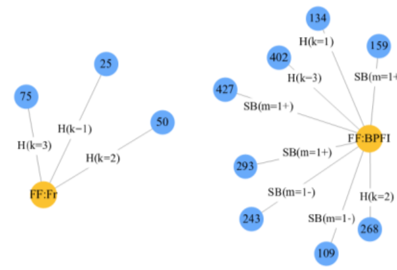
$$f_v = f_c \pm f_r \tag{7}$$

where f_r denotes the rotational frequency. These relations reflect frequency modulation structures generated by bearing fault mechanisms. By explicitly encoding harmonic and sideband dependencies, the constructed graph captures structured fault signatures rather than isolated amplitude variations.

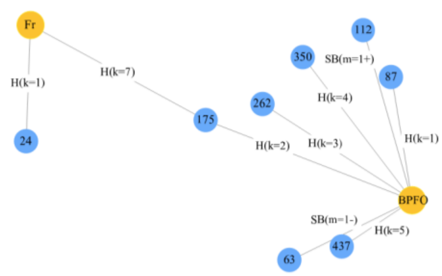
Through this process, the ontology-based frequency graph integrates spectral peaks, physically defined reference frequency components, and their relational structures into a unified representation. As illustrated in Figure 2, example graph maps for normal, inner-race fault, and outer-race fault samples highlight distinct harmonic and sideband patterns associated with each health condition. These structured graphs serve as the input to the subsequent GTN-based fault classification module.



(a) Normal condition graph map



(b) Inner condition graph map



(c) Outer condition graph map

Figure 2. Ontology-based frequency graphs for normal and fault conditions.

3.2. GTN-Based Fault Classification Module

The ontology-based frequency graph constructed in Section 3.1. serves as the structured input to the GTN classifier. The graph encodes frequency nodes, reference nodes, and typed harmonic and sideband edges, providing a physically grounded relational representation of bearing fault signatures. A GTN is then employed to learn composite meta-path structures over this heterogeneous graph, enabling the classifier to integrate fault evidence distributed across multi-hop relational paths.

Let $H^{(l)} \in \mathbb{R}^{|V| \times d_l}$ denote the node embedding matrix at layer l. After learning the composite adjacency matrix A_{meta}, graph convolution is applied to propagate node features as expressed in Eq. (8):

$$H^{(l+1)} = \sigma(A_{meta} H^{(l)} W^{(l)}) \tag{8}$$

where $W^{(l)}$ is a trainable weight matrix, and $\sigma(\cdot)$ denotes a nonlinear activation function. Through iterative propagation, node embeddings integrate information not only from directly connected neighbors but also from multi-hop relational paths induced by harmonic and sideband structures.

In particular, GTN learns structured interaction patterns such as frequency–reference–frequency associations and harmonic propagation chains, which correspond to physically meaningful fault signatures.

To make this concrete, a meta-path in the proposed graph is a composite relation obtained by chaining the harmonic and sideband edges through reference nodes. For example, the meta-path Frequency–(harmonic)–Reference–(harmonic)–Frequency links two spectral peaks that are both harmonics of the same characteristic frequency, such as the first and second harmonics of BPFO, thereby representing a harmonic family indicative of an outer-race fault. As a second example, the meta-path Frequency–(sideband)–Reference – (harmonic)–Frequency connects a sideband component to a harmonic of the same reference, capturing the joint harmonic–sideband modulation pattern characteristic of an inner-race fault, in which BPFI harmonics are flanked by sidebands spaced at the rotational frequency. By learning to weight such composite relations automatically, the GTN aggregates fault evidence along physically meaningful multi-hop paths. Unlike approaches that rely solely on isolated spectral amplitudes, this relational modeling framework enables the classifier to leverage structured dependencies among frequency components.

After L GTN layers, the final node embedding matrix $H^{(L)} = [h_1^{(L)}, h_2^{(L)}, \dots, h_{|V|}^{(L)}]$ encodes global relational information across the entire graph. To obtain a graph-level representation for classification, the node embeddings are aggregated using mean pooling as defined in Eq. (9):

$$h_G = \frac{1}{|V|}\sum_{v \in V} h_v^{(L)} \tag{9}$$

where $h_G \in \mathbb{R}^{d_g}$ denotes the graph embedding and $|V|$ is the total number of nodes. Mean pooling is adopted as a permutation-invariant aggregation function, ensuring that the graph representation is independent of node ordering.

The resulting graph embedding is passed through a fully connected classifier to produce the predicted fault label as defined in Eq. (10):

$$\hat{y} = f_{cls}(h_G) \tag{10}$$

where f_{cls} is implemented as a multilayer perceptron trained in a supervised manner. The model parameters are optimized end-to-end by minimizing the cross-entropy loss as defined in Eq. (11):

$$\mathcal{L} = -\sum_{c} y_c \log \hat{y}_c \tag{11}$$

where y_c denotes the ground-truth label. The complete diagnostic pipeline, from ontology-based graph construction to GTN-based classification, is evaluated under unseen domain conditions in the following section.

4. Experimental Validation

4.1. Experiment Setup

To validate OFG-GTN, experiments were conducted using three publicly available bearing datasets: the JNU Bearing Dataset, the MFPT Bearing Dataset, and the KAIST Bearing Dataset. These datasets encompass a wide range of fault types and operating conditions, providing a comprehensive foundation for evaluating diagnostic performance and generalization capability under unseen domain conditions. In this study, three health states are considered: healthy, outer-race fault, and inner-race fault. A summary of the datasets is presented in Table 1.

Table 1. Summary of dataset.

Case No.	Dataset	Load	RPM
1	JNU Bearing Dataset	–	600 / 800 / 1000
2	MFPT Bearing Dataset	22~136 N	1500
3	KAIST Bearing Dataset	0 / 2 / 4 Nm	3010

4.2. Analysis of Experimental Results

To assess the practical performance of OFG-GTN, comparative experiments were conducted against three baseline models selected to represent methodologically distinct approaches to cross-domain fault diagnosis. These baselines were chosen to cover representative strategies ranging from standard data-driven learning without domain generalization to feature-level domain alignment and optimization-based domain generalization. All baseline models receive FFT spectral features as input to ensure a fair and consistent comparison. The baselines include a conventional CNN classifier composed of stacked 1-D convolutional layers followed by max-pooling and fully connected layers, which serves as a standard data-driven reference without any domain generalization capability; Domain Adversarial Neural Network (DANN) (Ganin et al., 2016), which learns domain-invariant features through adversarial training between a feature extractor and a domain discriminator; and Meta-Learning for Domain Generalization (MLDG) (Li et al., 2018), which adopts a meta-learning strategy to explicitly optimize for generalization across unseen domains.

This study evaluates OFG-GTN under two complementary settings. The first is a standard in-domain classification setting, which serves as a reference: all three operating conditions are represented during training, and test samples are drawn from the same (seen) domains, so that the baseline classification capacity of each model can be assessed in the absence of domain shift. The corresponding results are reported in Table 2. The second is a leave-one-dataset-out cross-domain protocol, which constitutes the primary evaluation of generalization under domain shift. It is important to note that all three datasets share an identical label space comprising three health states (healthy, outer-race fault, and inner-race fault), so the classifier consistently predicts over the same set of fault categories in both settings; what varies across the cross-domain folds is solely the operating condition (load and rotational speed) and the data-acquisition system, that is, the input domain rather than the label set. In each cross-domain fold, one dataset is held out entirely as the unseen target domain, and the model is trained on only the remaining two source datasets, with no sample from the held-out domain used during training or validation. Accordingly, the cross-domain accuracy reflects classification over the same three known fault types using data acquired under an operating condition never observed during training, thereby directly quantifying robustness to domain shift rather than the recognition of previously unseen fault classes. This protocol reflects realistic deployment scenarios, in which a model trained on a limited set of conditions must remain reliable on machinery operating under conditions outside the training distribution; the corresponding results are reported in Table 3.

Under the standard in-domain setting, where no domain shift is present, all four models attain high and comparable classification accuracy, as summarized in Table 2. This confirms that the baseline models possess sufficient representational capacity for the bearing fault classification task itself, and that the performance differences observed under the cross-domain setting arise specifically from their differing ability to cope with domain shift rather than from limitations in nominal classification accuracy.

Table 2. Diagnostic accuracy (%) under the standard in-domain classification setting.

Method	Case 1	Case 2	Case 3
OFG-GTN	98.44	100	96.97
CNN	92.32	94.56	91.45
DANN	94.74	86.00	95.52
MLDG	88.52	91.00	93.75

As shown in Table 3 and Figure 3, OFG-GTN consistently achieves the highest diagnostic accuracy across all three cases, with approximately 90%, 93%, and 76% accuracy for Case 1, Case 2, and Case 3, respectively. In contrast, the baseline models exhibit substantially lower and less stable performance under unseen domain conditions. CNN and DANN show moderate accuracy in the range of 51–61% across cases, while MLDG demonstrates severe performance degradation particularly in Cases 2 and 3, dropping to approximately 23% and 22%, respectively. These results indicate that conventional data-driven and domain generalization approaches struggle to maintain diagnostic reliability when evaluated on unseen operating conditions, likely due to their reliance on statistical feature distributions that are susceptible to domain shift. In contrast, OFG-GTN, by grounding its representation in physical invariants of bearing fault mechanics through ontology-based graph construction, achieves consistent generalization across all unseen test domains.

Table 3. Diagnostic accuracy (%) under leave-one-out cross-domain evaluation.

Method	Case 1	Case 2	Case 3
OFG-GTN	90.00	93.26	75.75
CNN	61.52	54.34	60.97
DANN	51.52	52.05	60.97
MLDG	62.00	23.00	21.95

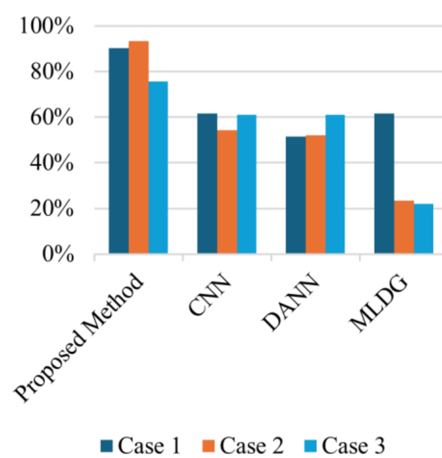


Figure 3. Performance under unseen domain conditions.

5. CONCLUSION

This study proposed OFG-GTN, an ontology-based bearing fault diagnosis framework in which vibration signals are reformulated as heterogeneous frequency graphs that explicitly encode the relational structure of bearing fault signatures. Rather than relying on statistical feature distributions that are susceptible to domain shift, OFG-GTN grounds its representation in analytically defined fault frequency relationships, and a GTN is employed to learn composite relational dependencies for graph-level classification. Evaluation under a leave-one-dataset-out cross-domain protocol demonstrated that OFG-GTN consistently outperformed conventional data-driven and domain generalization baselines across all unseen test domains, confirming that physics-informed relational representation is an effective and transferable basis for robust diagnosis. This property is also practically significant: field condition-monitoring data come from many assets that differ in equipment and operating conditions, which forces conventional models to be retrained with new labeled data for each unseen machine, load, or speed. By embedding domain knowledge directly into the representation, OFG-GTN can instead be applied to new equipment and operating conditions without such condition-specific retraining. As future work, we plan to integrate a large language model to interpret the graph-based diagnostic results, realizing an end-to-end ontology-based system that combines structured fault classification with natural language explanations.

ACKNOWLEDGEMENT

This research was supported by Basic Science Research Program through the National Research Foundation of Korea (NRF) funded by the Ministry of Education (RS-2025-25415980), and also supported by the Technology development Program (RS-2024-00487451) funded by the Ministry of SMEs and Startups (MSS, Korea).

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Yong Hun Park is currently enrolled in the integrated M.S.–Ph.D. program in Industrial Engineering at Ajou University. He received his B.S. degree in Industrial Engineering from Ajou University in 2024. His research interests include fault diagnosis and anomaly detection for rotating machinery, reliability analysis of semiconductor devices, and large language model (LLM)–based diagnostic frameworks. In particular, he focuses on developing interpretable and robust fault diagnosis methods under data-scarce conditions. He is currently conducting research at the Data Intelligent PHM Lab at Ajou University.

Seo Won Lee received her BSc degree in Mechanical Convergence Engineering from Konyang University in 2025. Since 2026, she has been pursuing a master's degree in Industrial Engineering at Ajou University. Her research interests broadly include fault diagnosis and condition monitoring of engineering systems, and she is currently exploring potential research topics in this area.

Chan Hee Park is currently an Assistant Professor in the Department of Mechanical and Information Engineering at the University of Seoul. She received her Ph.D. degree in Mechanical Engineering from Seoul National University. Prior to joining the University of Seoul, she worked as a staff engineer at Samsung Electronics. Her research focuses on domain generalization for robust fault diagnosis in rotating machinery and agent-based AI in manufacturing systems.

Joon Ha Jung is currently serving as an assistant professor of industrial engineering at Ajou University. He holds a BSc and a PhD in mechanical engineering from Seoul National University, which he obtained in 2012 and 2019, respectively. Prior to joining Ajou University, he worked as a senior researcher at the Korea Institute of Machinery and Materials (KIMM). Professor Jung's primary research focus is on fault diagnosis for rotating machinery, and he is also engaged in research activities that uses machine learning and deep learning.