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*Synergizing Quantum Chemistry and Machine  
Learning for Molecular Discoveries  
in the Condensed Phase*

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連絡先：化学研究所・分子材料化学研究領域 梶弘典（内線3149）

# Synergizing Quantum Chemistry and Machine Learning for Molecular Discoveries in the Condensed Phase

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## Abstract:

Machine learning (ML) and big data play increasingly critical roles in chemical discovery. However, datasets and ML models for condensed-phase molecular systems, such as solvated molecules and molecule assemblies, remain scarce. My research group leverages GPU-accelerated quantum chemistry and machine learning to address these gaps.

Many crucial solvent-solute interactions cannot be captured by the implicit solvent models routinely used in quantum chemistry calculation and require explicit solvent treatment. To streamline the simulation workflow for explicit-solvent calculations, we developed AutoSolvate, an open-source toolkit, which was later developed into a chatbot-assisted, cloud-based platform that automates simulation setup and execution using cloud computing resources. These tools have enabled the efficient generation of computational datasets for solvated molecules, which were used to train  $\Delta$ -ML models to enhance the accuracy of low-cost computational methods against experimental measurements. For molecular assemblies, we developed a size-transferable machine-learned exciton model to rapidly model their excited-state properties. More recently, we developed a domain-informed multi-agent AI framework that autonomously generates quantum-chemical training data, constructs molecule-specific machine-learned Hamiltonians and potential energy surfaces, and performs excited-state dynamics, with independent agents verifying scientific validity throughout the workflow.