Machine Learning for Tip Enhanced Raman Spectroscopy of Molecular Quantum Materials

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Molecular quantum materials promise transformative advances in quantum technologies, yet achieving their atomic-scale chemical insight remains a critical bottleneck. Tip-enhanced Raman spectroscopy (TERS) combines the high spatial resolution of scanning probe microscopy with the chemical specificity of Raman spectroscopy to overcome the Abbe diffraction limit, by exploiting a localized plasmonic "hot spot" at the tip apex [1]. However, interpreting TERS maps demands computationally intensive simulations [2] and expert analysis, impeding high-throughput studies. Building on our earlier automation of atomic force microscopy and scanning tunneling microscopy image analysis [3,4], we introduce a machine-learning framework trained on simulated TERS datasets to automate molecular structure characterization directly from TERS images. Our encoder–decoder architecture inputs frequency-resolved TERS intensity maps and rapidly predicts corresponding molecular geometries with high fidelity. Preliminary results demonstrate that our model reliably reconstructs key structural motifs across diverse small molecules, reducing analysis time by orders of magnitude while maintaining accuracy. By minimizing the reliance on resource-heavy simulations and expert-driven interpretation, this method paves the way for real-time, large-scale TERS characterization of complex molecular assemblies. Ultimately, our work will streamline the discovery and optimization of next-generation quantum materials, unlocking new pathways for device integration and fundamental studies at the molecular frontier.

Reference

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