DEPARTMENT OF CHEMISTRY AND ENVIRONMENTAL SCIENCE
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GUEST SPEAKER
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TOPIC
Quantum Machine Learning for Accurate and Low-Cost Computational Chemistry

ABSTRACT

Quantum mechanical predictions of ground-state and excited-state potential energy surfaces and properties face a punishing balance between prediction accuracy and computational cost, creating demand for new methods and modeling strategies. Machine learning (ML) for electronic structure offers promise in this regard, although conventional approaches require vast amounts of high-quality data and offer limited transferability in chemical space. We describe two frameworks for addressing this challenge: Molecular-Orbital-Based Machine Learning [1] and OrbNet [2]. These methods focus on training not with respect to atom-based features, but instead use features based on molecular orbitals, which have no explicit dependence on the underlying atom-types and thus provide greater chemical transferability. Both methods provide striking accuracy and transferability across chemical space while yielding 1000-fold or greater reductions in computational cost.

[1] "Improved accuracy and transferability of molecular-orbital-based machine learning: Organics, transition-metal complexes, non-covalent interactions, and transition states." Husch, Sun, Cheng, Lee, and Miller, JCP, 154, 064108 (2021).
[2] "OrbNet: Deep learning for quantum chemistry using symmetry-adapted atomic-orbital features. " Qiao, Welborn, Anandkumar, Manby, and Miller, JCP, 153, 124111 (2020).

BIO
Tom Miller is a scientist and entrepreneur with focus on the nexus of AI, chemistry, and biology. He joined the Caltech faculty in 2008 and was promoted to full professor in 2013. He's published more than 130 peer-reviewed articles and patents and received numerous awards for research excellence. Tom is co-founder and CEO of Entos, an AI-driven biopharma that recently closed a $53m Series A raise. The Entos team includes over 40 world-class AI researchers, software engineers, and scientists, and continues to grow.

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