

Showcasing research from Professor Weitang Li's laboratory, School of Science and Engineering, The Chinese University of Hong Kong, Shenzhen, China.

Quantum machine learning of molecular energies with hybrid quantum-neural wavefunction

Quantum computation and machine learning are revolutionizing computational chemistry because of their superior ability to represent and manipulate molecular wavefunctions. This work introduces a hybrid framework that learns molecular wavefunction using a combination of an efficient quantum circuit and a deep neural network. The results show not only high accuracy but also significant resilience to noise, highlighting the robustness of our method in practical quantum applications.

Image reproduced by permission of Weitang Li from *Digital Discovery*, 2025, **4**, 2697.



