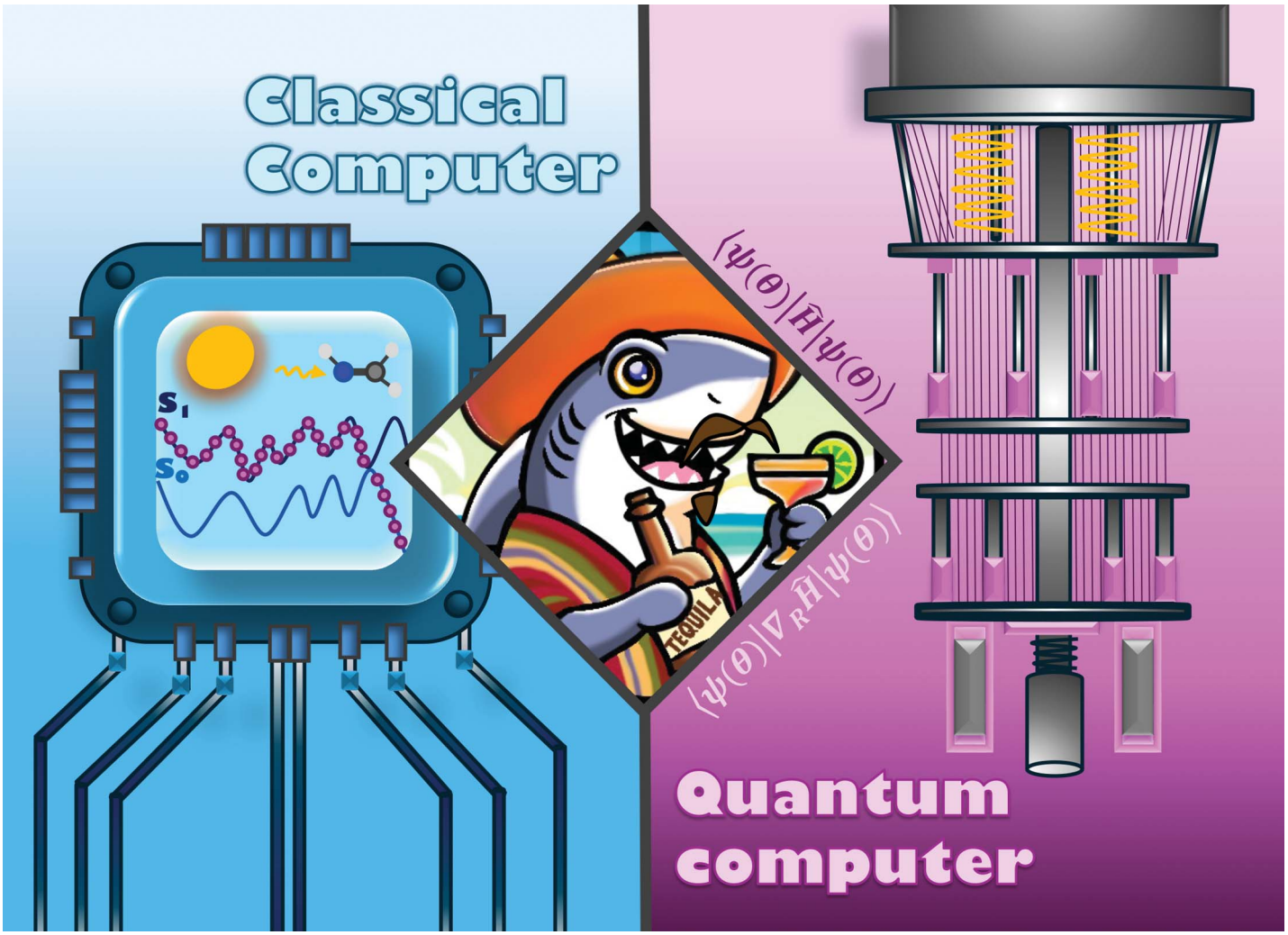

Showcasing research from Professor González Group, Institute of Theoretical Chemistry, Faculty of Chemistry, University of Vienna, Austria.

SHARC meets TEQUILA: mixed quantum-classical dynamics on a quantum computer using a hybrid quantum-classical algorithm

We present a hybrid quantum-classical approach that combines quantum and classical hardware to simulate the excited state dynamics of molecules. The method uses variational quantum eigensolver and variational quantum deflation algorithms to compute ground and excited state energies, gradients and couplings, which are then used to perform nonadiabatic dynamics using Tully's surface hopping method. This approach is implemented by integrating the SHARC molecular dynamics package with the TEQUILA quantum computing framework.

As featured in:

See Eduarda Sangiogo Gil, Leticia González *et al.*, *Chem. Sci.*, 2025, **16**, 596.

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