

Help chemists understand the practical advantages of quantum computers

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In recent years, quantum computing has emerged as a transformative tool in various scientific domains, particularly in chemistry. However, a significant gap persists between quantum computing and the chemistry community, primarily due to the complexities involved in translating chemical problems into a format amenable to quantum computation. In this presentation, we will first illustrate the practical advantages of quantum computers on chemical applications. We introduce the AutoCAS workflow on Azure Quantum Elements platform, designed specifically to aid chemists in navigating the intricate landscape of quantum computing. AutoCAS stands as a pioneering tool that enables chemists to assess whether the electronic structure problem that they encounter necessitates the use of quantum computing resources. More significantly, it automates the complex process of preparing inputs for quantum computers, thus democratizing access to quantum computing for chemists without requiring them to have extensive knowledge in quantum mechanics.