Quantum applied chemistry to benefit society

An interview with **Keeper Layne Sharkey**, Founder & Director at ODE, L3C --- Chair, Quantum Applied Chemistry at Quantum Security Alliance by Alain Chancé, CEO QUANTALAIN SASU.

Dr. Keeper Layne Sharkey

Keeper is **founder and director** at ODE, L3C, a for-profit, social enterprise venture that serves through Quantum Science, Technology and Research (qSTAR). Its aim is to change the world by solving NP Hard problems with **quantum computing**.

Keeper is **Chair, Quantum Applied Chemistry** at Quantum Security Alliance which was formed to bring academia, industry, researchers, and US government entities together to identify, define, collaborate, baseline, standardize and protect sovereign countries, society, and individuals from the far-reaching **impacts of Quantum Computing**.

Her skills and expertise include the following: Quantum Mechanics, Energy, Computational Chemistry, Density Functional Theory, Quantum Chemistry, Electronic Structure, Molecular Modeling, Molecular Dynamics, Physical Chemistry, Molecular Dynamics Simulation

Keeper's profile on LinkedIn, https://www.linkedin.com/in/klshark/

1/ What is your vision of quantum computing, quantum applied chemistry and their impact on society?

Society has a lot to gain from the computational capacity of tomorrow's quantum computer. Quantum computing will allow us to extract new knowledge from very large data sets provided that the mathematical equations used for predictive measures are accurately represented in the calculations and processed correctly by the quantum device. Ideally, this new knowledge will aid in fostering a wise and holistic community and has the real potential to change the world as we know it.

Regarding quantum applied chemistry, the major hurdle that needs to be overcome in order to realize accurate implementation of quantum chemistry is the Born-Oppenheimer approximation.

To elaborate: the BO world is one where electrons "see" or "experience" nuclei as having an infinite mass, a sort of black hole without complicated math - completely ignoring the nuclei's effect on all other particle interactions. Furthermore, this approximation assumes that the motions of the nuclei and the motions of the electrons are separable, and that the nuclei *do not behave quantum mechanically*, i.e., nuclei do not exhibit wave-like behavior. **This mass approximation has major consequences when trying to understand particle correlations. The effect not being accounted for is called mass polarization.** For more info on this topic see:
https://www.linkedin.com/pulse/accuracy-vs-assumption-quantum-age-where-chemistry-meets-sharkey

2/ What is your focus right now?

My main focus is a method I am calling QLEAN: Quantum Learned Electrons And Nuclei, i.e., not assuming the Born–Oppenheimer approximation, the assumption that the motion of atomic nuclei and electrons in a molecule can be treated separately. An innovative algorithm for quantum applied chemistry which does not assume the BO approximation is presented in the following two papers; one about atomic states and one about diatomic molecular states:

Atomic states: Keeper L. Sharkey, Nikita Kirnosov, and Ludwik Adamowicz, An algorithm for quantum mechanical finite-nuclear-mass variational calculations of atoms with L = 3 using all-electron explicitly correlated Gaussian basis functions, J. Chem. Phys. 138, 104107 (2013); https://doi.org/10.1063/1.4794192

Diatomic molecular states: Keeper L. Sharkey, Nikita Kirnosov, and Ludwik Adamowicz, Non-Born-Oppenheimer method for direct variational calculations of diatomic first excited rotational states using explicitly correlated all-particle Gaussian functions, PHYSICAL REVIEW A 88, 032513 (2013); https://doi.org/10.1103/PhysRevA.88.032513

3/ In which areas are you open for collaboration and joint ventures?

Running the above non BO algorithms on currently available quantum computers and quantum simulators, and well as advance qubit design at room temperature that does not require cooling.

I am also interested in fostering a quantum smart workforce through co-developing educational curriculum for both kids and adults and also contributing to the ethical practices regarding the implementation strategies of quantum technologies. I should emphasize that developing and fostering a quantum computing ontology with reasonable definitions without the use of superlatives should be a high priority within our community - so I would love to contribute there. With that said, having a well-defined definition of quantum computing itself should be a high priority to the industry so that we can better enable society to understand what it is and how we'll use it. The New York Times has recently asked promentient community members to define quantum computing and the responses were inconsistent to say the least, and in some cases downright whimsical.

I am also excited to broaden my horizon extending my joint venture to Europe and Partnering with Quantum World Association (QWA).

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