Cutting-edge technologies in computational chemistry

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Technology is revolutionizing the world and our daily lives. Over the years, the scientific progress greatly benefited by such technological explosion, and as new technologies continue to be developed, scientists will continue to adapt their workflows to the new available platforms.

In this contribution we combined cutting-edge technologies in machine learning, cloud computing and augmented reality to develop a series of interactive applications with the aim of making computational chemistry routinely accessible to the wider community.

We developed ChemVox[1], a free, ready-to-use Alexa skill that interfaces Amazon Web Services with the PubChem chemical database and the TeraChem Cloud[2] framework for cloud-based quantum chemistry. ChemVox is usable on all Alexa-capable devices and can answer questions related to the electronic properties of small- and medium-sized (up to ~100 atoms) molecules in a matter of seconds. This application offers easy access to quantum chemistry simulations for anyone with a smartphone.

Furthermore, we combined machine learning and augmented reality (AR) to develop MolAR, an immersive mobile application for visualizing molecules in real-world scenes [3]. The application uses deep learning to recognize hand-drawn hydrocarbons structures[4] which it converts into interactive 3D molecules in AR. MolAR was designed to be used in both research and education settings, providing an almost barrierless platform to visualize and interact with 3D molecular structures in a uniquely immersive way.

Lastly, we are developing a proof-of-concept implementation of a robot able to recognize chemical structures (by vocal or visual inputs), perform quantum-chemistry calculations and interact with the users.

In conclusion, we combined the most advanced and easily accessible technologies (e.g., virtual assistants, augmented reality and mobile devices) to make quantum chemistry a readily accessible tool for the community.

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