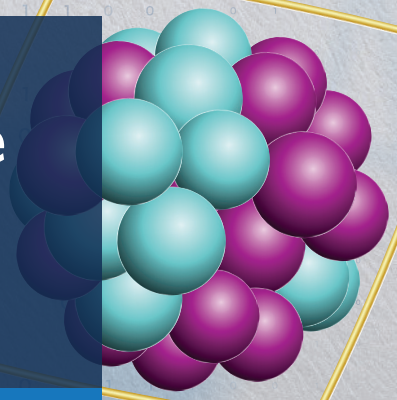
# Quantum Chemistry Promises to Advance AspenTech Process Optimization



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# Executive Overview

The Aspen Properties® database and supporting development tools have led the industry for the past 40 years in providing thermodynamic properties throughout the lifecycle of chemical processes. When the Aspen Properties capability first entered the market in 1983, the online availability of physical properties for chemistry and chemical engineering was an immediate game-changer for the discovery, development and operation of chemical processes. AspenTech has continued to lead in the application of digital physical properties through the constant addition of new property methods, innovations such as electrolyte properties systems, a strong partnership with the global research community through its close relationship with NIST, innovation in democratizing workflows for users to develop new properties correlations, and improving properties related to carbon capture amine systems. Most recently, AspenTech has introduced an increasingly rich set of properties data for bio-feedstock and bio-based chemicals modeling.

AspenTech has not only expanded the reach of Aspen Properties to support AspenTech software across all its simulation tools (Aspen Plus® family, Aspen HYSYS® family and Exchanger Design & Rating). It has gone beyond that to include the Aspen Unified PIMS™ environment, to create a consistent workflow between the design and digital twin environment, and operational planning and optimization systems.

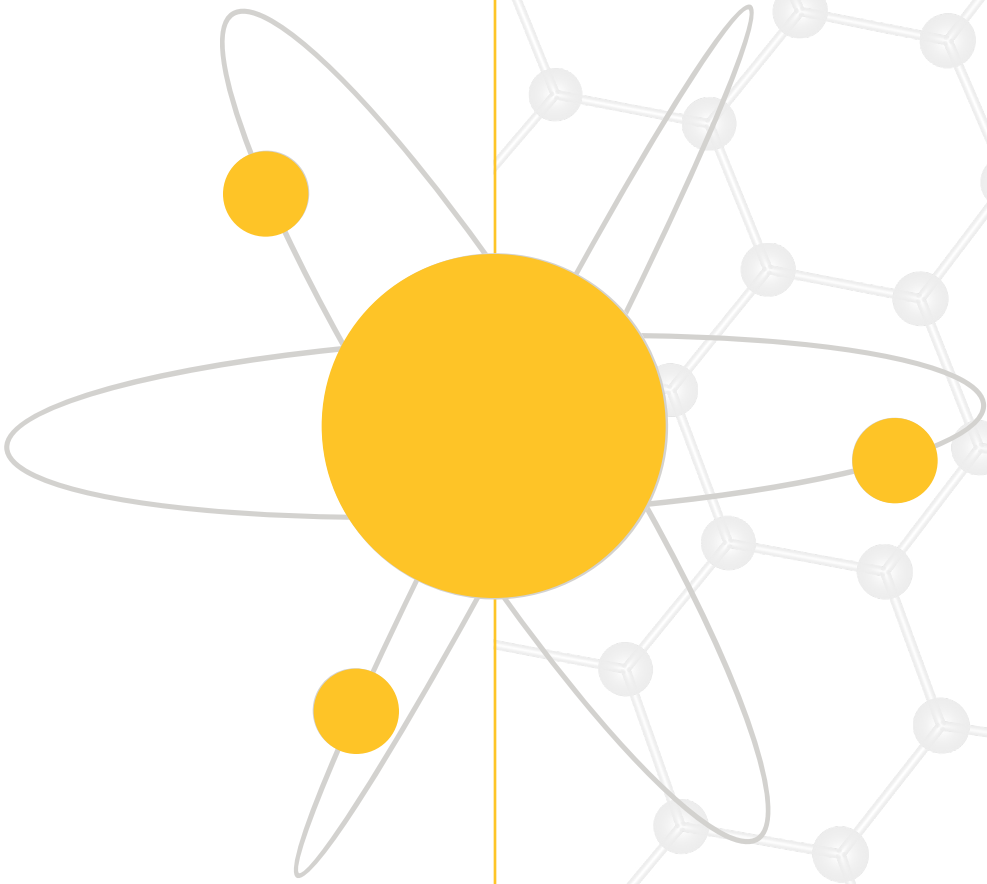
Now more than ever, with chemical engineering innovation focused on bio-based chemicals, oleochemistry, green cement and challenging new processes such as carbon capture, the ability to rapidly compute accurate thermodynamic properties for new chemicals is crucial for accelerating discovery, process technology development, and scale up of new processes and new materials.

Quantum chemistry methods have the potential to take the extremely strong foundation and industry-wide use of Aspen Properties to the next level as the world seeks to introduce new sustainable materials, processes, and industrial lifecycle approaches that can both drive towards zero carbon processes and support circularity strategies.

With the introduction of Microsoft Azure Quantum Elements in mid-2023, Microsoft and AspenTech announced a collaboration aimed at exploring avenues to take advantage of the combined strengths of AQE and Aspen

Properties. Microsoft and AspenTech believe that Azure Quantum Elements could be leveraged to develop a quantum chemistry workflow within Aspen Properties that could be extremely powerful and provide a unique new approach for estimating the thermodynamic properties for new molecules that are not currently available in the Aspen Properties database. This would offer a new means to rapidly develop thermodynamic parameters to support development of novel processes and new chemical products.

As a proof-of-concept, AspenTech and Microsoft used density functional theory (DFT), a quantum chemical simulation method, to estimate the heat of formation for a series of selected C6-C12 organic molecules. The results indicate that a quantum chemistry-based protocol, implemented by Microsoft in Azure Quantum Elements, derives accurate estimations, without the need for pre-trained parameters, such as the definition of the chemical groups in the group contribution method. Following this preliminary success, we are planning to further validate the quantum chemistry workflows as well as test pre-trained machine learning models, in order to assess a wider list of thermodynamic properties. Assuming that these proofs-of-concept are successful, AspenTech's vision is to make this capability available.  This will take advantage of the broad reach of Aspen Properties, making a quantum chemistry workflow with Microsoft AQE a strategic enabler. It would be available for the many types of innovation required across the energy, chemical, pharma and metals industries, enabling sustainable process industry, the broader energy transition movement, the introduction of new materials, and better circularity.

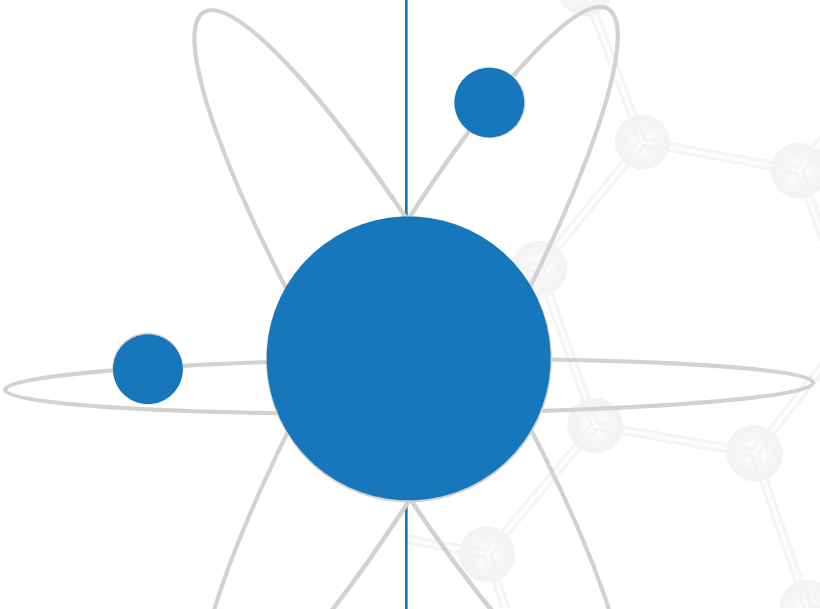


# Current Business Challenges

The 28th meeting of the Conference of the Parties (COP) in Dubai (December 2023) incorporated a landmark agreement of all signatory countries to move the world away from the use of fossil fuel in energy systems. This leaves the global economy with the dual challenge of a predicted growing demand for energy (30% by 2050), electricity (50% by 2050) and consumables (30% by 2050), with the ambition to achieve a net-zero carbon world by 2050. This is already driving the emergence of new energy sources, new chemical materials—some based on bio-feedstocks—new approaches to extracting green minerals such as lithium, and new carbon removal processes. To increase the scope and speed of innovation in a way that meets the world's ambitions, breakthroughs in chemical engineering, materials science and process technology are needed.

As a leader in chemical engineering and asset optimization, AspenTech has more than 40 years of experience in modeling large-scale processes efficiently in a wide range of industries. The key to successfully simulating the processes from first principles is to understand the atomistic-level interactions between chemical species, which are captured by the thermodynamic properties of each species, such as the chemical potential and the heat of formation.

For existing processes, AspenTech has a rich menu of databases and methods built in Aspen Properties that can support the simulations in Aspen Plus and Aspen HYSYS, and operations planning in Aspen Unified PIMS. However, the speed of development of new processes is already exceeding the expansion rate of high-quality physical property database additions, and process simulations therefore need new approaches to maintain and improve the accuracy of their predictions. A promising solution is to provide the end user with tool sets, such as quantum chemistry-based simulations, that can estimate the unknown thermodynamic properties with acceptable accuracy.

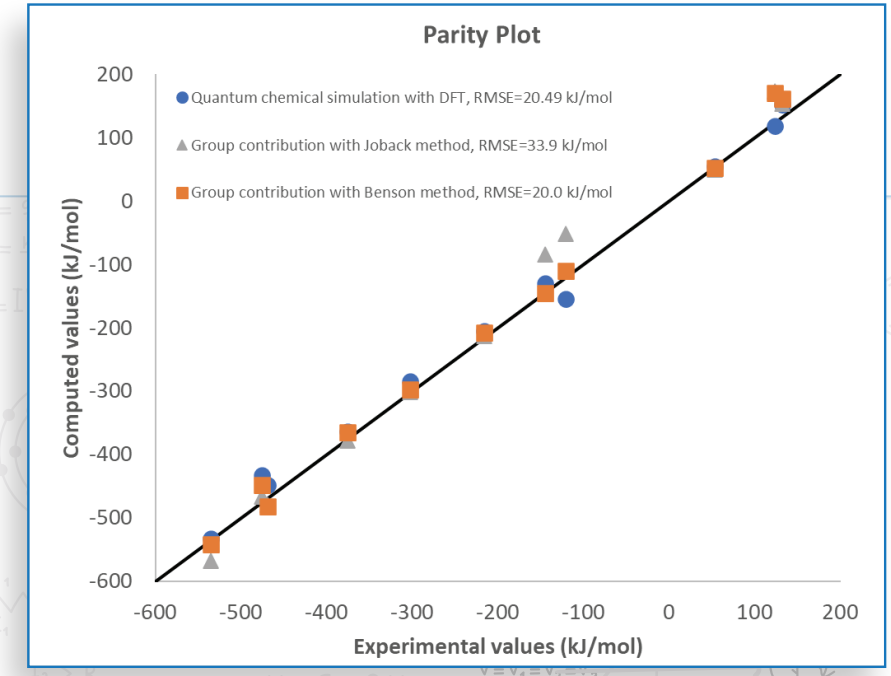


# Quantum Chemistry Estimates Heat of Formation

The Schrödinger Equation was proposed in the 1920s to describe the energy of a system from a quantized perspective. The formula was then applied in chemistry to depict the configuration and energy of the electrons and atoms in molecules, polymers and solid-state materials, thus establishing the field of quantum chemistry.

Among the list of thermodynamic properties used in process simulations, heat of formation is an ideal test case for evaluating the capabilities of quantum chemical tools. The heat of formation is the enthalpy difference of the molecule and its element references, where the enthalpy can be derived by the energy obtained from quantum chemistry simulations and thermodynamic principles.

The heat of formation can be assessed through the following steps:




1. Provide the molecule geometry, i.e., the coordinate of each atom.
2. Optimize the geometry with quantum simulations.
3. Obtain the energy of the optimized geometry.
4. Implement the thermodynamic principles to obtain the enthalpy correction and sum up with the energy in step 3 to obtain the enthalpy of the molecule.
5. Compute the energy of the elements in the form of a single atom and use the reference in literature to derive the enthalpy of each atom.
6. Take the enthalpy difference between steps 4 and 5 to derive the heat of formation of the molecule.

As a proof-of-concept, the heat of formation of a series of C6-C12 organic molecules was estimated with density functional theory (DFT), one of the quantum chemical simulation tools provided in Azure Quantum Elements, and the group contribution methods in literature. DFT simulations achieved 20 kJ/mol, which has similar accuracy to the estimation of the group contribution method in literature without parameter tuning beforehand.

## Vision of Quantum Chemistry in the Process Industry

Research in using quantum chemistry to estimate the chemical properties of molecules has been performed for decades, but commercial usage is prohibitive due to its demanding computational requirements. With the recent developments in the theory of quantum mechanics, simulation algorithms and computing power, the molecule size and estimation accuracy can now be performed faster and with better results than traditional approaches, eliminating previous barriers that stopped it from becoming important to the process industry.

Azure Quantum Elements is a purpose-built service on the Microsoft Azure platform that promotes scientific discovery and accelerates certain chemical simulations. The service employs open-source quantum chemical simulation packages such as NWChem and PySCF in high-performance computing (HPC) architecture.

Providing access to the Azure Quantum Elements service in AspenTech software can enable users to prepare a unique and accurate thermodynamic property database on top of Aspen Properties, allowing for efficient process simulations of the novel processes. Incorporating the Azure Quantum Elements property estimation application to achieve quantum chemistry adoption within the Aspen Properties thermodynamic database will enable the industry to accelerate discovery and innovation, and provide digital models for understanding the performance of these new chemicals and processes. It will result in accelerated scale-up and adoption, and optimize processes to improve economics and reduce carbon intensity.

## Conclusions

AspenTech and Microsoft are collaborating to design a quantum chemistry workflow that allows the user to estimate the thermodynamic property rapidly and confidently in the absence of experimental measurements. Our proof-of-concept shows that this approach can reach an accurate assessment in the example test, and we are continuing to test the approach with larger molecules. We believe this new tool can help users collect thermodynamic information, run process simulations with new molecules, and scale up processes with potential to tackle the dual challenge.

# Next Steps

AspenTech and Microsoft are investigating the possibility of estimating other essential thermodynamic properties with quantum chemistry. A series of workflows is envisioned once the methodology is proven for different types of molecules. The team is also investigating the use of pre-trained machine learning (ML) models as an alternative approach to predicting thermodynamic properties.

AspenTech aims to use quantum chemistry approaches for better characterization, process improvement, and faster introduction of new materials in the area of specialty chemicals such as advanced materials, new materials and pharmaceuticals.  Use cases we are focusing on include accelerating the development of new materials and processes, enhancing thermodynamic precision over other estimation methods, and improving process optimization. AspenTech is currently soliciting several key innovative "early adopter" companies to co-innovate with AspenTech and Microsoft in this area, with the goal of impacting the net zero and circularity goals of industrial companies.

**IMPORTANT NOTE:**

This white paper provides an AspenTech vision. There is currently no functionality in the quantum chemistry area described below that is either released or committed for future release.  This topic is still in the research phase.

## About Aspen Technology

Aspen Technology, Inc. (NASDAQ: AZPN) is a global software leader helping industries at the forefront of the world's dual challenge meet the increasing demand for resources from a rapidly growing population in a profitable and sustainable manner. AspenTech solutions address complex environments where it is critical to optimize the asset design, operation and maintenance lifecycle. Through our unique combination of deep domain expertise and innovation, customers in capital-intensive industries can run their assets safer, greener, longer and faster to improve their operational excellence.

**aspentech.com**

## About Microsoft

Microsoft (Nasdaq "MSFT" @microsoft) creates platforms and tools powered by AI to deliver innovative solutions that meet the evolving needs of our customers. The technology company is committed to making AI available broadly and doing so responsibly, with a mission to empower every person and every organization on the planet to achieve more.

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