Rolf Lustig

DR.-ING. HABIL. ROLF LUSTIG received his Diploma from the University of Hannover in 1981 and his doctorate from Ruhr-University Bochum in 1985, both in Mechanical Engineering. After a two-year postdoctoral appointment in the Chemistry Department of Pennsylvania State University, he returned to a faculty position at the Institute of Physical Chemistry at Aachen University of Technology (RWTH Aachen) in Germany.

He successfully finalized his Habilitation in Physical Chemistry in 1994, leading to the highly prestigious Heisenberg Fellowship Award from the German Research Foundation in 1995. The Award came with a five-year sabbatical leave from his faculty position at RWTH.

Dr. Lustig spent this time to deepen his understanding of the fundamentals in his field of expertise, Statistical Thermodynamics. Most of his work during this period was conducted again at Penn State. In 2000, he decided to stay in the United States for family reasons and accepted a faculty position as an Assistant Professor in the Department of Chemical and Biomedical Engineering at Cleveland State University. Dr. Lustig was promoted through the ranks to Professor.

Dr. Lustig's main interests are in the application of his expertise to Molecular Simulation. Over the past decades, this field has evolved from being an academic luxury to serious attempts to replace costly laboratory experiments on the thermophysical properties of matter by numerical experiments on High Performance Computing (HPC) systems.

In this method, a system of about a thousand model molecules are moved around in a virtual box to mimic real molecular behavior.

During his time at CSU, Dr. Lustig has developed novel, rigorous methodologies to measure the entirety of thermodynamic properties simultaneously in a single molecular simulation. As a result, complete equations of state can be simulated in a matter of weeks, as opposed to decades in an actual laboratory.

He takes pride that these methodologies led to the first computer-generated equation of state with an accuracy high enough to serve as scientific standard. This work was done in an international collaboration with two German research groups and was published in the Journal of Physical and Chemical Reference Data in 2016.

There are many by-products of Dr. Lustig's work in the fundamentals of Statistical Thermodynamics. He has published several highly cited papers on pure mathematics. Recently, a highly accurate and purely theoretical equation of state for atomic solids has been derived by him. Sophisticated data correlation methods for thermodynamic properties are another active field of his research.

As a curiosity, Dr. Lustig's research partners in Germany hold the world record for the largest molecular system ever simulated: twenty trillion particles on one of the most powerful HPC systems in the world. Dr. Lustig himself holds the world record for the smallest system ever simulated: Three atoms were shown to undergo a solid-fluid phase transition on his modest computing equipment at CSU.

This was his latest work published before his retirement from higher education. It will certainly not be his last.