**Machine-Learning Models of Potential Energy Surfaces as a Tool for Understanding Structure and Reactivity – Prof. Dr. Jeremy Harvey**

This presentation explores the application of machine-learning (ML) models to study molecular structures and chemical reactivity through the construction of potential energy surfaces (PES). We employ neural network-based ML potentials enhanced with equivariant transformations to improve both efficiency and accuracy.

In one approach, a difference-learning strategy is applied to semi-empirical density functional theory (DFT) data to produce a high-fidelity model approximating accurate DFT results. This model enables exhaustive conformational searches for complex macrocyclic compounds of biological relevance.

In a second approach, the ML model learns the PES of a model ATP hydrolysis and synthesis reaction (hydrolysis of methyl pyrophosphate) in explicit water. This allows detailed investigation of the mechanism and dynamics of the reaction in a realistic solvent environment.

These examples demonstrate how ML-derived PES models can accelerate understanding of both structural landscapes and reactive processes, bridging computational efficiency with chemical accuracy.

**Curriculum vitae of Prof. Dr. Jeremy Harvey**

Jeremy Harvey was born in the UK in 1969 and moved to Belgium as a child. He obtained a Licentiate (1990) and Doctorate (1995) in Chemistry from UC Louvain, Louvain-la-Neuve. Following his doctorate in experimental organic chemistry, he completed two postdoctoral fellowships in Berlin, Germany and Jerusalem, Israel, during which he transitioned to computational and theoretical chemistry.

He began his independent research career in Bristol, UK (1999–2014) and has been at KU Leuven since 2014, where his work focuses on using quantum-chemistry-based computational techniques to understand chemical reaction mechanisms and dynamics. Since 2020, he has also served as Head of the Department of Chemistry at KU Leuven.