



Harish-Chandra Research Institute



# Infosys Lecture Series

## Energy landscapes: from molecules and nanodevices to machine learning

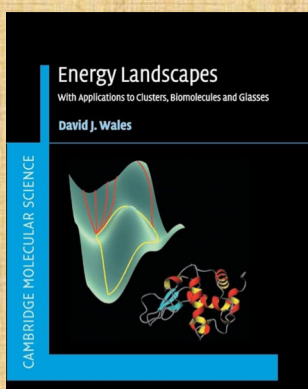


Venue: HRI Auditorium  
Prayagraj, India

Time: 4:30pm (IST)  
Date: 22<sup>nd</sup> – 24<sup>th</sup> April, 2024

**Prof. David Wales (FRS), University of Cambridge, U.K.**

**Infosys Distinguished Visiting Professor, HRI Prayagraj, India**



**ABSTRACT:** The potential energy landscape provides a conceptual and computational framework for investigating structure, dynamics and thermodynamics in atomic and molecular science. These lectures will summarise recent developments for global optimisation, quantum dynamics, the thermodynamic properties of systems exhibiting broken ergodicity, and rare event dynamics. Applications will be presented that range from prediction and analysis of high-resolution spectra, to coarse-grained models and design principles for self-assembly of mesoscopic structures, with recent results for machine learning landscapes and first passage time distributions.

