

The Warsaw Doctoral School in Natural and Biomedical Sciences and the Institute of Physics PAS cordially invites you to a **SPOTLIGHT TALK**

Energy Landscapes: New Horizons

given by

Prof. David J. Wales

Cambridge University

on 30th October 2024, 12:00 at the IP PAS Auditorium

Duration: 45 min + question time

The event will be available on ZOOM also, at this link

All Warsaw-4-Phd students (and others) very welcome!

Abstract of the talk:

The potential energy landscape provides a conceptual and computational framework for investigating structure, dynamics and thermodynamics in atomic and molecular science.

This lecture will summarise recent developments for global optimisation, enhanced sampling, and rare event dynamics.

A variety of recent applications will be presented including proteins, nucleic acids, coarse-grained models, and design principles for self-assembly of mesoscopic structures, with recent results for global kinetics based on first passage time distributions.

Selected Publications:

Nat. Commun (2024) 15, 8763. Design principles for energy transfer in the photosystem II supercomplex from kinetic transit ion networks.

J. Phys. Chem. B (2024) 128, 7568. Vibrational Energy Landscapes and Energy Flow in GPCRs

Perspective: Journal of Physical Chemistry Letters (2022) 13, 6349. Dynamical Signatures of Multifunnel Energy Landscapes

Ann. Rev. Phys. Chem., 69, 401-425, (2017). Exploring Energy Landscapes

Chem. Commun, 53, 6974-6988 (2017). Exploring biomolecular energy landscapes

Energy Landscapes: Some New Horizons, Curr. Op. Struct. Biol., 20, 3-10, 2010.

Energy Landscapes, Cambridge University Press, Cambridge, 2003

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David J. Wales received his BA degree from Cambridge University in 1985, PhD in 1988, and ScD in 2004. He was a Lindemann Trust Fellow in 1989, a Research Fellow at Downing College Cambridge in 1990, a Lloyd's of London Tercentenary Fellow in 1991, and a Royal Society University Research Fellow from 1991 to 1998. In 1998 he was appointed to a Lectureship in Cambridge and is now Professor of Chemical Physics and Chair of the Theory group. He was awarded the Cambridge University Norrish Prize for Chemistry and the Gonville and Caius College Schuldham Plate in 1985, the Meldola Medal and Prize in 1992 and the Tilden Prize in 2015, both by the Royal Society of Chemistry. He was a Baker Lecturer at Cornell University in 2005, the Inaugural Henry Frank Lecturer at the University of Pittsburgh in 2007, Distinguished Lecturer at the National Institute of Standards and Technology, USA in 2018, and was awarded a Visiting Miller Professorship at the University of California, Berkeley, for 2020. He was elected a Fellow of the Royal Society in 2016. In 2020 he became the inaugural recipient of the ICRéDD Award from Hokkaido University and received a Humboldt Research Prize from the Alexander von Humboldt Foundation. He is an Honorary Professor at the University of Warwick for 2022-2025, Infosys Distinguished Visiting Professor, Harish-Chandra Research Institute, Allahabad, 2023, and Distinguished Visiting Professor, New York University, 2024. His research primarily involves the exploration of energy landscapes, with applications to chemical biology, spectroscopy, machine learning, clusters, solids and surfaces.