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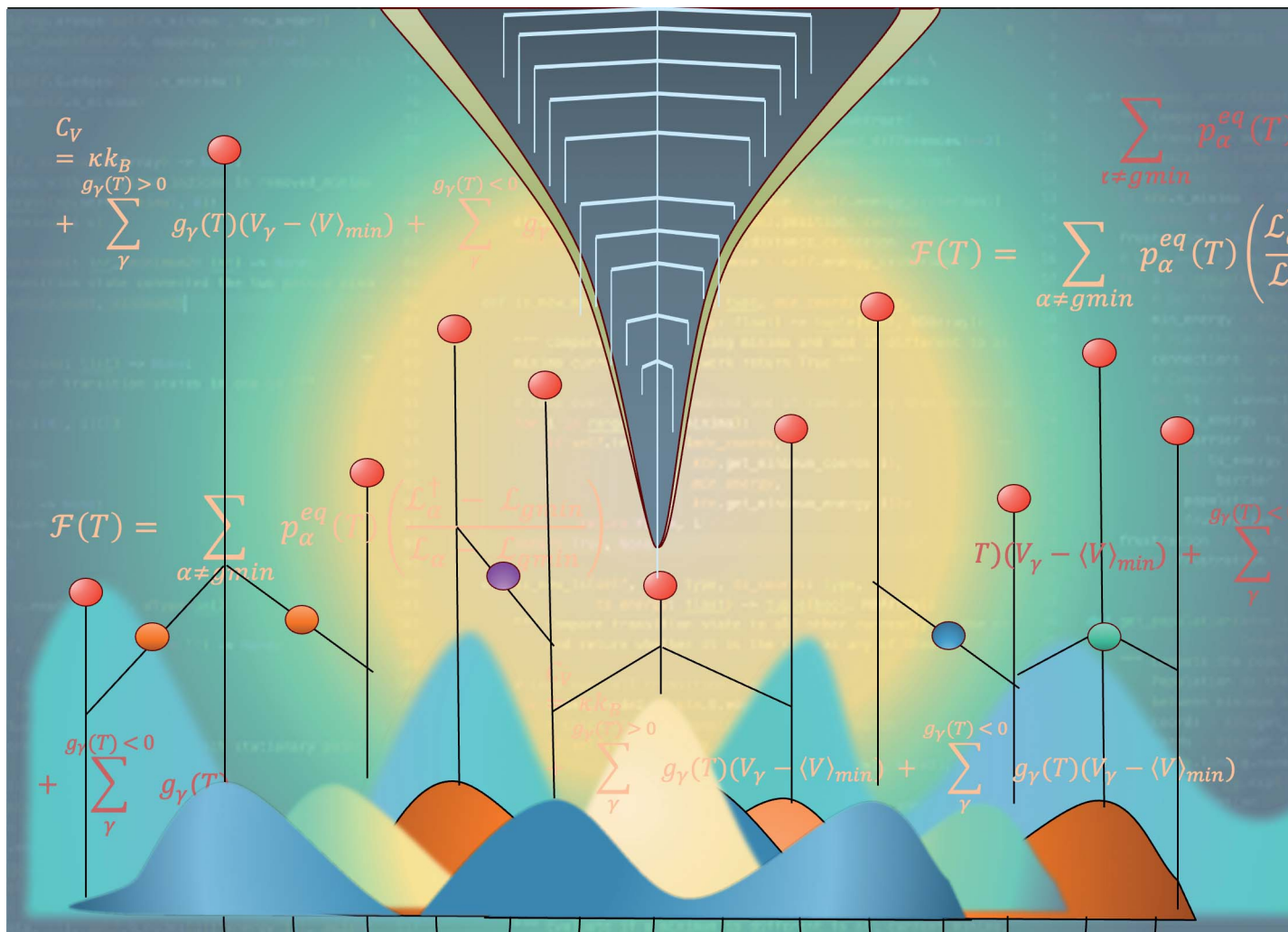


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Showcasing research from the collaboration between the groups of Professor Wales - Yusuf Hamied, Department of Chemistry, University of Cambridge, and Dr Pyzer-Knapp - IBM Research Europe.

Insights into machine learning models from chemical physics: an energy landscapes approach (EL for ML)

This work showcases how principles from Chemical Physics, namely the Energy Landscapes approach, can be applied to machine learning models. We show how various physical properties find analogues in machine learning systems, and how these properties can be employed to both increase understanding of the machine learning 'black-box' and enhance the performance of machine learning models.

As featured in:



See Edward O. Pyzer-Knapp, David J. Wales *et al.*, *Digital Discovery*, 2024, 3, 637.