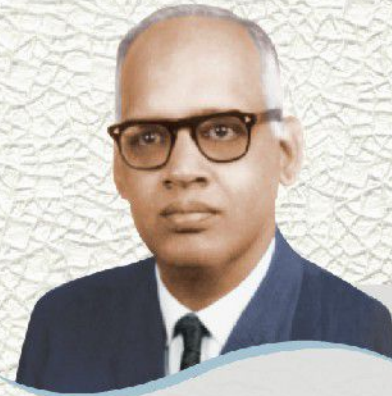


Professor Daan Frenkel: Brief Profile



Professor Daan Frenkel, FRS, is a world leader in numerical simulations in diverse areas ranging from soft matter, biological to chemical Systems. He is renowned for explaining several phenomena related to phase transitions — changes of state — in 'soft matter' such as polymers, colloids and gels. Amongst many applications, Daan's techniques can be used to help understand the behaviour of cell membranes, in order to advance medical science. In living organisms, proteins perform a multitude of functions. In order to work out their structure, researchers grow 'crystals' from solutions of purified proteins. His simulations reveal promising new ways to make tiny holes in materials — 'nano scale pits' — that enable the rapid growth of high- quality protein crystals. He has been influential in fostering and promoting computer-based research. He is the co-author of *Understanding Molecular Simulation* (2001), a widely used handbook for computational physicists. Daan has received numerous awards, including the 2007 Aneesur Rahman Prize for Computational Physics of the American Physical Society, and the 2007 Alder–CECAM Prize of the European Physical Society.



5th

G. N. Ramachandran Memorial Lecture

on

*Counting the Uncountable:
Entropy, granular Entropy and Information*

by

Professor Daan Frenkel

Department of Chemistry, University of Cambridge, UK

Thursday, 13th February, 2020 at 3:30 pm

in

Silver Jubilee Hall,

SNBNCBS



S. N. Bose National Centre for Basic Sciences
Block- JD, Sector- III, Salt Lake
Kolkata - 700 106

**Counting the Uncountable:
Entropy, granular Entropy and Information**

Professor Daan Frenkel

ABSTRACT

In an attempt to construct a Statistical Mechanics of Powders, Sir Sam Edwards introduced the concept of "granular entropy", defined as the logarithm of the number of distinct packings of N granular particles in a fixed volume V . In 1989, the proposal was rather controversial but much of the debate was sterile because the granular entropy could not even be computed for systems as small as 20 particles - hardly a good approximation of the thermodynamic limit.

In my talk I will describe how granular entropies of much larger systems can now be computed, using a novel algorithm. Interestingly, it turns out the definition of granular entropy will have to be modified to guarantee that granular entropy is extensive. Which brings us back to the Gibbs paradox and a little-discussed secret of colloid science.



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On behalf of Staff & Students of the Centre
I cordially invite you to the

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Prof. Samit Kumar Ray
Director

