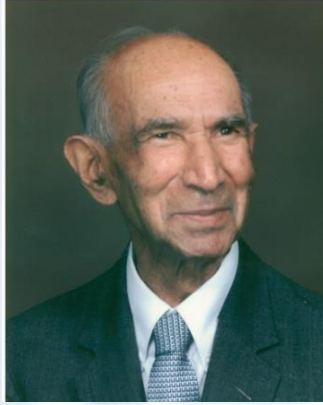


# Department of Physics, Panjab University, Chandigarh

## *8<sup>th</sup> Prof. B.M. Anand Lecture*



Prof. Bal Mokand Anand was history's choice for establishing Panjab University's Physics Department in its permanent campus at Chandigarh and initiating research activity here. He published original research in the 1930s and 1940s and had the distinction of working for his doctorate, in the 1950s, under the supervision of Professor Cecil Frank Powell who had been awarded physics Nobel Prize in 1947 for the discovery of pion (or pi meson), using nuclear emulsion technique. Anand's 20-page research paper, based on his Ph. D. work, and published by the Royal Society, London, in 1953 is still considered relevant. Bal Mokand was born in a village, Domel, in the Bannu district of what is now the Khyber Pakthunwa province of Pakistan. B M Anand was appointed as Lecturer in 1934. Professor B M Anand headed Physics Department for two terms 1953-1963 and 1964-1967. He retired from Panjab University in 1967.

## **Prof. B.M. Anand**

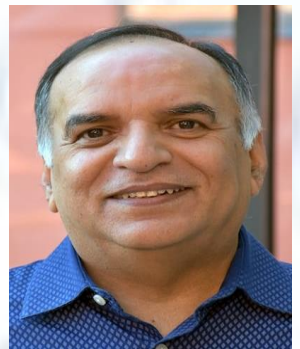
(1905 – 1998)

**SPEAKER**

*Prof. Rajeev Ahuja, Director, IIT, Ropar & Professor, Uppsala University, Sweden*

*Speaks on*

**“Computational materials science and its applications in the area of materials for energy”**



### **Abstract:**

Energy storage has been a theme for scientists for two hundred years. The Lead acid battery research on batteries occupied some of the best minds of the 19th century. Gaston Plante in 1859 invented the lead acid battery which starts your car and ignites the internal combustion which takes over the propulsion. Although the lead battery is over 150 years old but the origin of its open circuit voltage (OCV) of 2.1 V is still known. In present talk, I will show how one can explain the origin of OCV of 2.1 V based on foundations of relativistic quantum mechanics. Surprisingly, seems to be the first time its chemistry has been theoretically modeled from the first principles of quantum mechanics. The main message of this work is that most of the electromotoric force (1.7-1.8 Volts out of 2.1 V) of the common lead battery comes from relativistic effects. While the importance of relativistic effects in heavy-element chemistry is well-known since over two decades, this is a striking example on "everyday relativity". We believe that the fact that "cars start due to relativity." The purpose of this talk is to provide an overview of the most recent studies in the field of hydrogen storage materials & rechargeable battery research with the focus how computational material science can play an important role in search and design of new hydrogen storage materials & next generation battery materials. On specific examples, the application of density functional theory calculations and molecular dynamics simulations will be illustrated to show how these computational methods can be of great use in the effort to reach a better understanding of materials and to guide the search for new promising candidates.

### **About the Speaker:**

The eighth Prof. B. M. Anand Memorial Lecture is being delivered by Prof. Rajeev Ahuja. He is a professor of computational Materials science at Uppsala University, Sweden. Currently, he is serving as the Director of Indian Institute of Technology (IIT) Ropar, India. He was also holding the additional charge of director of IIT Guwahati, India from Nov. 2023 to May 2024. He is one of the most highly cited researchers as well as top 5 materials scientist in Sweden and India. He has done his Ph.D. from IIT Roorkee in India in 1992. Same year, he joined Uppsala University, Sweden as postdoctoral fellow. He became Professor in 2007 at Uppsala University, Sweden. His main area of interest is materials science with focus on energy such Batteries, Hydrogen Storage & production, sensors as well high-pressure physics. He has published 1150 scientific papers in peer reviewed journals H-Index of 105, i-10 index 809 & no. of citations more than 50000. Prof. Ahuja has supervised 30 PhD students, more than 35 post-docs.

**Awards:** Prof Ahuja has received several prestigious awards, including the Beller Lectureship at the APS March Meeting in 2017, the Wallmark Prize in 2011 from the Royal Swedish Academy of Sciences (KVA), and the Eder Lilly & Sven Thureus Prize, as well as the Benzelius Prize from the Swedish Royal Society of Sciences (KVS). He is an elected member of the Swedish Royal Society of Sciences (KVS). Prof Ahuja has been awarded Best Alumnus award from IIT Roorkee, India for excellence in research for 2021.

**Professional Recognition:** He has recently elected as the Fellow of the Royal Society of Chemistry (F-RSC), UK, and as an APS Fellow by the American Physical Society (APS), USA. He serves on the advisory board of the Journal of Materials Chemistry A and Materials Advances from the Royal Society of Chemistry. Additionally, he is the Associate Editor of Nano Energy.

**Venue: Prof. B.M. Anand Auditorium, Dept. of Physics, Panjab University.**

**Date: 5<sup>th</sup> November, 2024**

**Time: 11:00 am**