

E OF SCIENCE & TECHNOLOGY

ACCMS-Global Research Center, SRMIST, Chennai India Webinar #6

<u>Prof. D. D. Sarma</u>

Solid State and Structural Chemistry Unit Indian Institute of Science, Bengaluru, India

<u>Title:</u> Designing the smallest bandgap ferroelectric material

22nd February 2022, 10.00 – 11.30 am IST

Registration link: https://tinyurl.com/2p8wr2md

Biography

Prof. D.D. Sarma received his Ph.D. from Indian Institute of Science (IISc), Bangalore under the mentorship of highly renowned solid-state chemist, Prof. C. N. R. Rao. After a short stint as a guest scientist at Forschungszentrum, Julich, Germany, he returned to IISc in 1986 to start his independent career, where he has continued to date. Along with a Honorary Professorship at IISc, he has held additional honorary appointments at several national and international institutes. He has won several prestigious awards, including Sir. J. Ghosh Medal, young scientist award, C.V. Raman award, TWAS physics prize, the Shanti Swarup Bhatnagar Prize, Knight of the Order of the Star of Italy, the Firodia Award, the UNESCO Javed Hussain Prize, and the inaugural J. N. Tata Chair Professorship. Also, he has been elected as a fellow of all three Indian science academies and the national engineering academy, and he is a Fellow of the American Physical Society, a J. C. Bose National Fellow, and a Fellow of the Asia Pacific Academy of Materials. He has published several papers with the citations more than 23000 and h-index 81. He holds many patents. Prof. Sarma's career has been defined by his clarity of thought, love for teaching, and eye for detail that have invariably brought out the rich science hidden beneath every problem that he tackles. Last year, a special issue was published through 'Journal of Physical Chemistry C' as a 'Tribute to Prof. Sarma' for his contribution in the interdisciplinary area of condensed matter science, ranging from solid state chemistry to spectroscopy, physics of materials, and nanoscience, in the overarching theme of electronic structure.

<u>Abstract</u>

A low band gap ferroelectric material with a sizable polarization at ambient conditions would constitute an ideal photovoltaic material to harvest solar energy owing to their efficient polarization driven charge carrier separation as well as generation of high, above band gap, photovoltage upon photoexcitation. Consequently, these materials in principle can overcome what is normally considered as the maximum theoretical limit of photoconversion efficiency. Unfortunately, all known ferroelectric materials tend to have very high bandgap with little overlap with the solar spectrum and the consequent inability to absorb most of the solar spectrum. Design and synthesis of reduced band gap ferroelectric transition metal oxides without compromising their polarization properties has been a longstanding challenge with little success. Based on our recent work, I shall discuss how one may achieve this elusive goal by co-doping a Jahn-Teller Mn³⁺ and Nb⁵⁺ pair for two Ti⁴⁺ ions, representing a charge-neutral dipole doping, in ferroelectric BaTiO₃, achieving for the first time a bulk ferroelectric oxide with the lowest bandgap of 1.66 eV with a sizable polarization of nearly 70% of BaTiO₃. More recently, we have found theoretical indications to expand this strategy with co-doping of Cu²⁺ and Te⁶⁺ at the Ti⁴⁺ sites of BaTiO₃. Conveners

Zoom meeting details will be shared with the registered participants

Dr. V.J.Surya and Dr.S. Yuvaraj ACCMS-GRC Center-in-Charges Department of Physics and Nanotechnology, SRMIST-KTR

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