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LIST OF PUBLICATIONS

1. T. K. Kundu, S. Mishra, N. Karak, **P. Barik**, “Effect of Ti^{4+} ions doping on microstructure and dc resistivity of nickel ferrites”, **Journal of Physics and Chemistry of Solids**, 73, 2012, pp. 579–583.
2. **P. Barik**, A. Jana and T. K. Kundu, “Influence of Co – ion doping on tetragonal – orthorhombic polymorphic transformation and dielectric behavior in $BaTiO_3$ nanoparticles”, **Journal of American Ceramic Society**, 94, 2011, pp. 2119–2125.
3. T. K. Kundu, N. Karak, **P. Barik** and S. Saha, “Optical properties of ZnO nanoparticles prepared by chemical method using polyvinyl alcohol (PVA) as capping agent”. **International Journal of Soft Computing and Engineering**, 1, 2011, pp. 19-24.
4. **P. Barik**, T. K. Kundu and S. Ram, “Light emission from ferroelectric barium titanate nanocrystals”, **Philosophical Magazine Letters**, 89, 2009, pp. 545–555.
5. T. K. Kundu, A. Jana and **P. Barik**, “Doped barium titanate nanoparticles”, **Bulletin of Material Science**, 31, 2008, pp. 501–505.

PAPERS PRESENTED IN INTERNATIONAL/NATIONAL CONFERENCES

6. “Optical and Electrical Properties of CdS Quantum Dots embedded in Barium Titanate Matrix”, **P. Barik** and T. K. Kundu, *13th National Symposium in Chemistry (NSC-13)*, 4th-6th February, 2011.
7. “Photoluminescence of Doped Nano Barium Titanate”, T. K. Kundu and **P. Barik**, *International Conference on Nanotechnology & Medical Sciences (ICNAMS-2010)*, 21th-23th October, 2010.
8. “Doped $BaTiO_3$ nanoparticles”, T. K. Kundu, A. Jana and **P. Barik**, *Review and Coordination meeting on Nanoscience and Nanotechnology held at ARCI-Hyderabad (INDIA)*, 2007.

Abbreviation

	A-E		
<i>ac</i>	Alternating Current	<i>LEEM</i>	Low-Energy Electron Microscopy
<i>AES</i>	Auger Electron Spectroscopy	<i>LEELS</i>	Low Energy Electron Loss Spectroscopy
<i>AFM</i>	Atomic Force Microscopy	<i>MOCVD</i>	Metal Organic Chemical Vapor Deposition
<i>BT</i>	Barium Titanate	<i>NIR</i>	Near Infrared
<i>CET</i>	Cooperative Energy Transfer	<i>NNI</i>	National Nanotechnology Initiative
<i>DFWM</i>	Degenerate Four Wave Mixing	<i>NMR</i>	Nuclear Magnetic Resonance
<i>dc</i>	Direct Current	<i>NSOM</i>	Near-Field Scanning Optical Microscope
<i>EDS/EDX</i>	Energy-Dispersive X-Ray Spectroscopy	<i>OSL</i>	Optically Stimulated Luminescence
<i>eV</i>	Electron Volt		
<i>ESA</i>	Excited State Absorption		P-T
<i>ESCA</i>	Electron Spectroscopy For Chemical Analysis	<i>ps</i>	Picosecond
<i>EPR</i>	Electron Paramagnetic Resonance	<i>PL</i>	Photoluminescence
<i>ESR</i>	Electron Spin Resonance	<i>PT</i>	Lead Titanate
<i>EELS</i>	Electron Energy Loss Spectroscopy	<i>RHEED</i>	Reflection High-Energy Electron Diffraction
	F-J	<i>ST</i>	Strontium Titanate
<i>FTIR</i>	Fourier Transform Infrared Spectroscopy	<i>STEM</i>	Scanning Transmission Electron Microscopy
<i>HRTEM</i>	High-Resolution Transmission Electron Microscopy	<i>SEM</i>	Scanning Electron Microscopy
<i>HRSEM</i>	High-Resolution Scanning Electron Microscopy	<i>SERS</i>	Surface Enhanced Raman Spectroscopy
<i>IR</i>	Infrared Spectroscopy	<i>STM</i>	Scanning Tunnelling Microscope
	K-O	<i>TEM</i>	Transmission Electron Microscopy
<i>KT</i>	Potassium Tantalate	<i>TL</i>	Thermoluminescence
<i>nm</i>	Nanometer		U-Z
<i>nc-BT</i>	Nanocrystalline-Barium Titanate	<i>XPS</i>	X-Ray Photoelectron Spectroscopy
μm	Micrometer	<i>XRD</i>	X-ray Diffraction
<i>LEED</i>	Low-Energy Electron Diffraction	<i>YAG</i>	Yttrium Aluminium Garnet