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1. Facet dependent catalytic activities of anatase TiO₂ for CO₂ adsorption and conversion. SB Mishra, BRK Nanda. Applied Surface Science 531, 147330.
2. Metal-insulator transition in epitaxial Ga-doped ZnO films via controlled thickness. J Mukherjee, BRK Nanda, MSR Rao. Journal of Physics: Condensed Matter.
3. Density Functional Theory Studies of Si₂BN Nanosheets as Anode Materials for Magnesium-Ion Batteries. P Panigrahi, SB Mishra, T Hussain, BRK Nanda, R Ahuja. ACS Applied Nano Materials 3 (9), 9055-9063.
4. Electronic Structure of Graphene/TiO Interface: Design and Functional Perspectives. SB Mishra, SC Roy, BRK Nanda. arXiv preprint arXiv:2007.14174.
5. Fluorine intercalated graphene: Formation of a two-dimensional spin lattice through pseudoatomization. SB Mishra, SK Yadav, DG Kanhere, BRK Nanda. Physical Review Materials 4 (7), 074411.
6. Pressure and Inversion Symmetry Breaking Field Driven First Order Phase Transition and Formation of Dirac Circle in Perovskites. A Kore, R Kashikar, M Gupta, P Singh, BRK Nanda. arXiv preprint arXiv:2004.06939.
7. Defining the topological influencers and predictive principles to engineer the band structure of halide perovskites. R Kashikar, M Gupta, BRK Nanda. Physical Review B 101 (15), 155102.
8. Mechanistic Understanding of NO₂ Dissociation on a Rutile TiO₂ (110) Surface: An Electronic Structure Study. S Marutheeswaran, SB Mishra, SC Roy, BRK Nanda. The Journal of Physical Chemistry C 124 (16), 8786-8794.
9. Maximizing Short Circuit Current Density and Open Circuit Voltage in Oxygen Vacancy-Controlled Bi_{1-x}Ca_xFe_{1-y}Ti_yO_{3-δ} Thin-Film Solar Cells. S Nandy, K Kaur, S Gautam, KH Chae, BRK Nanda, C Sudakar. ACS Applied Materials & Interfaces 12 (12), 14105-14118.
10. Band engineering via grain boundary defect states for large scale tuning of photoconductivity in Bi_{1-x}Ca_xFe_{1-y}Ti_yO_{3-δ}. S Nandy, PSV Mocherla, K Kaur, S Gautam, BRK Nanda, C Sudakar. Journal of Applied Physics 126 (23), 235101.
11. Localization Crossover Near Metal-Insulator Transition in Two-Dimension Limit of CaCu₃Ru₄O₁₂. S Jana, SG Bhat, BC Behera, L Patra, PS Kumar, BRK Nanda, D Samal. arXiv preprint arXiv:1908.11128.
12. Enhanced bulk photovoltaic response in Sn doped BaTiO₃ through composition dependent structural transformation. L Kola, D Murali, S Pal, BRK Nanda, P Murugavel. Applied Physics Letters 114 (18), 183901.
13. Large Bulk Photovoltaic Response by Symmetry-Breaking Structural Transformation in Ferroelectric (Ba (Zr 0.2 Ti 0.8) O 3-0.5 (Ba 0.7 Ca 0.3) Ti O 3). AB Swain, D Murali, BRK Nanda, P Murugavel. Physical Review Applied 11 (4), 044007.
14. Shifting of Fermi level and realization of topological insulating phase in the oxy fluoride BaBiO₂F. B Khamari, BRK Nanda. Materials Research Express 6 (6), 066309.

15. Stretchable and dynamically stable promising two-dimensional thermoelectric materials: ScP and ScAs. K Kaur, D Murali, BRK Nanda. *Journal of Materials Chemistry A* 7 (20), 12604-12615.
16. Unravelling Giant Exchange bias in the single layered Ruddlesden-Popper compound $\text{SrLaCo}_{0.5}\text{Mn}_{0.5}\text{O}_4$: A combined studies of Experimental and Density. RR Das, P Parida, AK Bera, T Chatterji, BR Nanda, S Nagappan Nair. *APS* 2019, L40. 011.
17. Second-neighbor electron hopping and pressure induced topological quantum phase transition in insulating cubic perovskites. R Kashikar, B Khamari, BRK Nanda. *Physical Review Materials* 2 (12), 124204.
18. Mn substitution controlled Li-diffusion in single crystalline nanotubular LiFePO_4 high rate-capability cathodes: Experimental and theoretical studies. AK Budumuru, M Viji, A Jena, BRK Nanda, C Sudakar. *Journal of Power Sources* 406, 50-62.
19. Universality in the electronic structure of 3d transition metal oxides. P Parida, R Kashikar, A Jena, BRK Nanda. *Journal of Physics and Chemistry of Solids* 123, 133-149.
20. Quantum-mechanical process of carbonate complex formation and large-scale anisotropy in the adsorption energy of CO_2 on anatase TiO_2 (001) surface. SB Mishra, A Choudhary, SC Roy, BRK Nanda. *Physical Review Materials* 2 (11), 115801.
21. Oxygen vacancy induced photoconductivity enhancement in $\text{Bi}_{1-x}\text{Ca}_x\text{FeO}_{3-\delta}$ nanoparticle ceramics: A combined experimental and theoretical study. S Nandy, K Kaur, PSV Mocherla, BRK Nanda, C Sudakar. *Journal of Applied Physics* 124 (19), 195108.
22. Giant exchange bias in the single-layered Ruddlesden-Popper perovskite. RR Das, P Parida, AK Bera, T Chatterji, BRK Nanda, PN Santhosh. *Physical Review B* 98 (18), 184417.
23. Quantum well structure of a double perovskite superlattice and formation of a spin-polarized two-dimensional electron gas. S Samanta, SB Mishra, BRK Nanda. *Physical Review B* 98 (11), 115155.
24. Giant photovoltaic response in band engineered ferroelectric perovskite. S Pal, AB Swain, PP Biswas, D Murali, A Pal, BRK Nanda, P Murugavel. *Scientific reports* 8 (1), 1-7.
25. Designing Nonpolar Metallic Interfaces using Insulating Transition Metal Olivine Phosphates. A Jena, D Murali, BRK Nanda. *Advanced Theory and Simulations* 1 (2), 1700007.
26. Topologically invariant double Dirac states in bismuth-based perovskites: Consequence of ambivalent charge states and covalent bonding. B Khamari, R Kashikar, BRK Nanda. *Physical Review B* 97 (4), 045149.
27. Microstrain engineered magnetic properties in $\text{Bi}_{1-x}\text{Ca}_x\text{Fe}_{1-y}\text{Ti}_y\text{O}_{3-\delta}$ nanoparticles: deviation from Néel's 1/d size-dependent magnetization behaviour. PSV Mocherla, MB Sahana, R Gopalan, MSR Rao, BRK Nanda. *Materials Research Express* 4 (10), 106106.

28. Effect of frustrated exchange interactions and spin-half-impurity on the electronic structure of strongly correlated. NiFeO₄ K Ugendar, S Samanta, S Rayaprol, V Siruguri, G Markandeyulu. Physical Review B 96 (3), 035138.
29. Virtual synthesis of crystals using *ab initio* MD: Case study on LiFePO₄. SB Mishra, BRK Nanda. AIP Conference Proceedings 1832 (1), 090044.
30. Metal-Insulator Transition in Ga doped ZnO via Controlled Thickness. J Mukherjee, BRK Nanda, MS Rao. arXiv preprint arXiv:1704.03846.
31. Microstrain induced deviation from Néel's 1/d behaviour: Size-dependent magnetization in Bi_{1-x}CaxFe_{1-y}TiyO_{3-δ} nanoparticles. PSV Mocherla, MB Sahana, E Abdelhamid, D Hajra, B Nadgorny, R Naik. arXiv preprint arXiv:1703.07190.
32. Orbital driven impurity spin effect on the magnetic order of quasi-3D cupric oxide. BG Ganga, PN Santhosh, BRK Nanda. Journal of Physics: Condensed Matter 29 (15), 155802.
33. Engineering diffusivity and operating voltage in lithium iron phosphate through transition-metal doping. A Jena, BRK Nanda. Physical Review Applied 7 (3), 034007.
34. Enhancing CO₂ Electroreduction by Tailoring Strain and Ligand Effects in Bimetallic Copper–Rhodium and Copper–Nickel Heterostructures. T Adit Maark, BRK Nanda. The Journal of Physical Chemistry C 121 (8), 4496-4504.
35. Microstrain induced deviation from Néel's 1/d behaviour: Size-dependent magnetization in Bi_{1-x}CaxFe_{1-y}TiyO_{3-δ} nanoparticles. PSV Mocherla, MB Sahana, E Abdelhamid, D Hajra, B Nadgorny, R Naik. arXiv, arXiv: 1703.07190.
36. Quantum confinement in double perovskite multilayers: Sr₂FeMoO_{6/La2}CoMnO₆. S Samanta, B Nanda. APS 2017, R43. 004.
37. Thickness driven metal-insulator transition in PLD grown Ga doped ZnO thin films: experiment and first principle studies. J Mukherjee, BRK Nanda, MS Rao. APS 2017, T1. 070.
38. Orbital driven impurity spin effect on the magnetic order of quasi-three dimensional cupric oxide. BG Ganga, PN Santhosh, BRK Nanda. arXiv preprint arXiv:1610.00458.
39. First principles study of the electronic structure and magnetic properties of spin chain compounds: Ca₃ZnMnO₆ and Ca₃ZnCoO₆. J Chakraborty, S Samanta, BRK Nanda, I Dasgupta. Journal of Physics: Condensed Matter 28 (37), 375501.
40. Tailoring p-and n-type semiconductor through site selective oxygen doping in Cu₃N: density functional studies. G Sahoo, R Kashikar, MK Jain, BRK Nanda. Materials Research Express 3 (6), 065902.
41. Magnetism in intercalated graphene. S Ali, BRK Nanda. AIP Conference Proceedings 1731 (1), 130040.
42. CO and CO₂ Electrochemical Reduction to Methane on Cu, Ni, and Cu₃Ni (211) Surfaces. T Adit Maark, BRK Nanda. The Journal of Physical Chemistry C 120 (16), 8781-8789.

43. Intertwined lattice deformation and magnetism in monovacancy graphene. H Padmanabhan, BRK Nanda. *Physical Review B* 93 (16), 165403.
44. Spin-glass state in nanoparticulate $(\text{La}_{0.7}\text{Sr}_{0.3}\text{MnO}_3)_{1-x}(\text{BaTiO}_3)_x$ solid solutions: Experimental and density-functional studies. C Nayek, S Samanta, K Manna, A Pokle, BRK Nanda, P Murugavel. *Physical Review B* 93 (9), 094401.
45. Unconventional Magnetism and Band Gap Formation in LiFePO_4 : Consequence of Polyanion Induced Non-planarity. A Jena, BRK Nanda. *Scientific reports* 6, 19573.
46. Control over the charge transfer in dye-nanoparticle decorated graphene. SR Bongu, AV Veluthandath, BRK Nanda, S Ramaprabhu, PB Bisht. *Chemical Physics Letters* 644, 176-182.