

P Murugan, CECRI.

1. Structural evolution, electronic and physicochemical properties of tin ozonide nanoclusters: a density functional theory perspective. OK Akiode, P Murugan, AI Adeogun, GA Adebayo, MA Idowu. *Journal of Nanoparticle Research* 22 (9), 1-11.
2. Enhancing Hydrogen Evolution Reaction Activities of 2H-Phase VS<sub>2</sub> Layers with Palladium Nanoparticles. K Karthick, TK Bijoy, A Sivakumaran, AB Mansoor Basha, P Murugan. *Inorganic Chemistry* 59 (14), 10197-10207.
3. Rational Design of Highly Efficient Perovskite Hydroxide for Electrocatalytic Water Oxidation. SR Ede, TK Bijoy, SS Sankar, P Murugan, S Kundu. *Inorganic Chemistry* 59 (7), 4816-4824.
4. Atomic and electronic structure of solids of Ge<sub>2</sub>Br<sub>2</sub>PN, Ge<sub>2</sub>I<sub>2</sub>PN, Sn<sub>2</sub>Cl<sub>2</sub>PN, Sn<sub>2</sub>Br<sub>2</sub>PN and Sn<sub>2</sub>I<sub>2</sub>PN inorganic double helices: a first principles study. TK Bijoy, P Murugan, V Kumar. *RSC Advances* 10 (25), 14714-14719.
5. V<sup>3+</sup> Incorporated  $\beta$ -Co(OH)<sub>2</sub>: A Robust and Efficient Electrocatalyst for Water Oxidation. S Anantharaj, K Karthick, P Murugan, S Kundu. *Inorganic Chemistry* 59 (1), 730-740.
6. Effect of anionic and cationic substitutions on the magnetic property of hydrated  $\alpha$ -MnO<sub>2</sub>. G Kruthika, P Ravindran, P Murugan. *AIP Conference Proceedings* 2115 (1), 030490.
7. Structure-magnetic property relations in FeNbO<sub>4</sub> polymorphs: A spin glass perspective. N Lakshminarasimhan, AKN Kumar, SS Chandrasekaran, P Murugan. *Progress in Solid State Chemistry* 54, 20-30.
8. Lithiation of the Two-Dimensional Silicon Carbide–Graphene van der Waals Heterostructure: A First Principles Study. TK Bijoy, P Murugan. *The Journal of Physical Chemistry C* 123 (17), 10738-10745.
9. Integration of phenylammoniumiodide (PAI) as a surface coating molecule towards ambient stable MAPbI<sub>3</sub> perovskite for solar cell application. KO Ogunniran, G Murugadoss, R Thangamuthu, J Karthikeyan. *Solar Energy Materials and Solar Cells* 191, 316-328.
10. Computational Approach To Reveal the Structural Stability and Electronic Properties of Lithiated M/CNT (M= Si, Ge) Nanocomposites as Anodes for Lithium-Ion Batteries. TK Bijoy, P Murugan. *ACS omega* 4 (2), 4153-4160.
11. Fluorine-enriched mesoporous carbon as efficient oxygen reduction catalyst: understanding the defects in porous matrix and fuel cell applications. V Parthiban, B Bhuvaneshwari, J Karthikeyan, P Murugan, AK Sahu. *Nanoscale Advances* 1 (12), 4926-4937.
12. d z<sup>2</sup> orbital-mediated bound magnetic polarons in ferromagnetic Ce-doped BaTiO<sub>3</sub> nanoparticles and their enriched two-photon absorption cross-section. P Senthilkumar, S

- Dhanuskodi, J Karthikeyan, P Murugan. *Physical Chemistry Chemical Physics* 21 (7), 4032-4045.
13. Real-time decay of fluorinated fullerene molecules on Cu (001) surface controlled by initial coverage. AI Oreshkin, DA Muzychenko, SI Oreshkin, VA Yakovlev, P Murugan. *Nano Research* 11 (4), 2069-2082.
  14. Borophene layers on an Al (111) surface—the finding of a borophene layer with hexagonal double chains and B 9 nonagons using ab initio calculations. J Karthikeyan, YS Ranawat, P Murugan, V Kumar. *Nanoscale* 10 (36), 17198-17205.
  15. Unveiling the multifunctional roles of hitherto known capping ligand oleic acid as blue emitter and sensitizer in tuning the emission colour to white in red-emitting phosphors. S Sekar, JG Muller, J Karthikeyan, P Murugan, N Lakshminarasimhan. *Physical Chemistry Chemical Physics* 20 (28), 19087-19097.
  16. Atomic structure and electronic properties of  $A_2B_2XY$  ( $A = \text{Si-Pb}$ ,  $B = \text{Cl-I}$ , and  $XY = \text{PN and SiS}$ ) inorganic double helices: first principles calculations. TK Bijoy, P Murugan, V Kumar. *Physical Chemistry Chemical Physics* 20 (15), 10060-10068.
  17. Growth Mechanism of Pine-leaf-like Nanostructure from the Backbone of  $\text{SrCO}_3$  Nanorods using LaMer's Surface Diffusion: Impact of Higher Surface Energy ( $\gamma = 38.9 \text{ eV/nm}^2$ ). D Arumugam, M Thangapandian, JL Joshua Mathavan, A Jayaram. *Crystal Growth & Design* 17 (12), 6394-6406.
  18. Structural and electronic properties of solid-state  $(\text{LiMPO}_4)_x(\gamma\text{-Li}_3\text{PO}_4)_y$  [010] electrochemical interface ( $M = \text{Fe and Co}$ ). SS Chandrasekaran, P Murugan *Applied Surface Science* 418, 17-21.
  19. Computational investigation on structural and electronic properties of various metal complexes of (2, 2'; 6', 2', 2''-terpyridine)-4-mercaptobenzoic acid ligand. TK Bijoy, A Palaniappan, P Murugan. *Applied Surface Science* 418, 275-279.
  20. Surface termination dependent atomic relaxation of  $\text{RT}_5$  ultra-thin slabs ( $R = \text{Y, Ce, Sm}$  and  $T = \text{Fe, Co, Ni}$ ) and their electronic and magnetic properties. SS Chandrasekaran, P Murugan, P Saravanan. *Applied Surface Science* 418, 291-295.
  21. Exploring the mechanism of spontaneous and lithium-assisted graphitic phase formation in SiC nanocrystallites of a high capacity Li-ion battery anode. TK Bijoy, J Karthikeyan, P Murugan. *The Journal of Physical Chemistry C* 121 (28), 15106-15113.
  22. Manifestation of Concealed Defects in  $\text{MoS}_2$  Nanospheres for Efficient and Durable Electrocatalytic Hydrogen Evolution Reaction. SM Senthil Kumar, K Selvakumar, J Karthikeyan, R Thangamuthu. *ChemistrySelect* 2 (17), 4667-4672.
  23. In-situ conversion of multiwalled carbon nanotubes to graphene nanosheets: an increasing capacity anode for Li Ion batteries. I Elizabeth, BP Singh, TK Bijoy, VR Reddy, G Karthikeyan, VN Singh. *Electrochimica Acta* 231, 255-263.
  24. Effect of ablation rate on the microstructure and electrochromic properties of pulsed-laser-deposited molybdenum oxide thin films. S Santhosh, M Mathankumar, S Selva Chandrasekaran. *Langmuir* 33 (1), 19-33.

25. Excitation-dependent local symmetry reversal in single host lattice Ba<sub>2</sub>A(BO<sub>3</sub>)<sub>2</sub>: Eu<sup>3+</sup> [A= Mg and Ca] phosphors with tunable emission colours. S Jayakiruba, SS Chandrasekaran, P Murugan, N Lakshminarasimhan. *Physical Chemistry Chemical Physics* 19 (26), 17383-17395.
26. Tuning of intrinsic antiferromagnetic to ferromagnetic ordering in microporous  $\alpha$ -MnO<sub>2</sub> by inducing tensile strain. G Kruthika, J Karthikeyan, P Murugan. *Physical Chemistry Chemical Physics* 19 (5), 3770-3776.
27. Magnetic and electronic properties of hard| soft magnetic interface in (YCo<sub>5</sub>| Co)[0001] and (YFe<sub>5</sub>| Co)[0001] superlattices. SS Chandrasekaran, MR Ponnaiah, P Murugan, P Saravanan. *Journal of Magnetism and Magnetic Materials* 418, 92-98.
28. Magnetic, thermodynamic and transport properties of novel non-centrosymmetric RCoSi<sub>3</sub> (R= Pr, Nd and Sm) compounds. S Nallamuthu, SS Chandrasekaran, P Murugan, M Reiffers. *Journal of Magnetism and Magnetic Materials* 416, 373-383.
29. Corrosion inhibition effect of novel methyl benzimidazolium ionic liquid for carbon steel in HCl medium. P Kannan, J Karthikeyan, P Murugan, TS Rao, N Rajendran. *Journal of Molecular Liquids* 221, 368-380.
30. A comparative study on electrochemical cycling stability of lithium rich layered cathode materials Li<sub>1-x</sub>Ni<sub>x</sub>M<sub>1-x</sub>O<sub>2</sub> where M= Fe or Co. CP Laisa, AKN Kumar, SS Chandrasekaran, P Murugan. *Journal of Power Sources* 324, 462-474.
31. Diverse spectroscopic studies and first-principles investigations of the zinc vacancy mediated ferromagnetism in Mn-doped ZnO nanoparticles. R Ponnusamy, SC Selvaraj, M Ramachandran, P Murugan *Crystal Growth & Design* 16 (7), 3656-3668.
32. First principles calculations on oxygen vacant hydrated  $\alpha$ -MnO<sub>2</sub> for activating water oxidation and its self-healing mechanism. K Ganesan, P Murugan. *Physical Chemistry Chemical Physics* 18 (32), 22196-22202.
33. First principles modeling of Mo<sub>6</sub>S<sub>9</sub> nanowires via condensation of Mo<sub>4</sub>S<sub>6</sub> clusters and the effect of iodine doping on structural and electronic properties. I Laraib, J Karthikeyan, P Murugan. *Physical Chemistry Chemical Physics* 18 (7), 5471-5476.