

**Dr. Rita John**

Professor

Department of Theoretical Physics,

University of Madras,

Guindy Campus, Chennai – 600 025.

Cell: 9566245138

E-mail: ritajohn.r@gmail.com

**Last 5 years publication list**

1. Manikandan Balakrishnan and Rita John, Properties of sol-gel synthesized multiphase TiO<sub>2</sub> (AB)-ZnO (ZW) semiconductor nanostructure: An effective catalyst for methylene blue dye degradation Iranian Journal of Catalysis, 10(1), 1-16, 2020.
2. J. Bhavani and Rita John, Band Gap Engineering of Cu<sub>2</sub>ZnSnX<sub>4</sub> (X = S, Se and Te) Quaternary Semiconductors Using PBE-GGA, TB-mBJ and mBJ+U Potentials, International Journal of Materials, Mechanics and Manufacturing, Vol. 8, No. 1, 2020.
3. S Padmavathi, Rita John, Spin polarized first principles calculations on electronic, magnetic and optical properties of Zn (1– x) AxS (A= Cr/Mn/Fe) using mBJ approximation,, Materials Science and Engineering: B, 248, 114401, 2019.
4. Namitha Anna Koshi, Rita John First principles study on the structural, electronic, magnetic and thermoelectric properties of CoX' NbGa (X'= Cr, Mn, Fe) quaternary Heusler alloys, , The European Physical Journal B, 92 (4), 86, 2019.
5. J. Bhavani, Rita John, Band Gap Engineering of Cu<sub>2</sub>-II-IV-VI<sub>4</sub> Quaternary Semiconductors Using PBE-GGA, TB-mBJ and mBJ+U Potentials, International Journal of Scientific Research in Physics and Applied Sciences, Vol.7, Issue.1, pp.65-75, 2019,
6. Manikandan, B., Endo, T., Kaneko, S., Murali, K.R., John, R, Properties of sol gel synthesized ZnO nanoparticles Journal of Materials Science: Materials in Electronics, 29(11), 9474-9485, 2018.
7. S. Padmavathi and Rita John, Investigation on Thermoelectric Properties of Wurtzite ZnO using modified Becke Johnson potential: a DFT study, International Journal of Current Advanced Research, Vol. 7, Issue 2(J), pp. 10266-10268, 2018.
8. Koshi,N.A., John, R., Half-Metallic Ferrimagnetism in CoFeNbZ (Z = Al, Si, Ge, Sn) Quaternary Heusler Alloys: a DFT Study, Journal of Superconductivity and Novel Magnetism, 32 (4), 977-986, 2018.
9. S. Padmavathi and Rita John, Study of Thermoelectric Properties of Zn<sub>1-x</sub>TM<sub>x</sub>S (TM=Cr/Mn/Fe) Systems using SpinPolarized Density Functional Theory, International Journal for Research in Applied Science and Engineering Technology, Vol. 6, Issue III, 2018.
10. R John, B Merlin, Ab initio calculation on the Optical Properties of AA-Stacked two-dimensional Graphene, Silicene, Germanene, and Stanene, International Journal of Computational Physics Series, 1 (1), 46-50, 2018
11. S. Padmavathi and Rita John Effect of Ternary Additions X (Co, Rh, Ir) on Electronic Properties of TiPd Shape Memory Alloy: An ab-initio Study,, International Journal for Research in Applied Science & Engineering Technology (IJRASET), Volume 6 Issue III, March, 2018.
12. John,R., Merlin, B Optical properties of graphene, silicene, germanene, and stanene from IR to far UV – A first principles study, Journal of Physics and Chemistry of Solids, 110, 307-315, 2017.

13. . R John, NA Koshi Band Jahn Teller Like Distortion In TiPd Shape Memory Alloy On Addition Of Magnetic Impurity Co, *Procedia Engineering*, 4 (4), 5185-5189,2017.
14. C., John, R., Murali, Dhanemozhi, , K.R., Synthesis and characterization of ZnS<sub>x</sub>Se<sub>1-x</sub> films using Brush plating technique, *Materials Today: Proceedings*, 4 (4), 5185-5189, 2017.
15. Rita John, B. Benita Merlin, Theoretical Investigation on 2D Materials: Graphene, Silicene, Germanene, and Stanene., *Journal of Materials Sciences & Engineering*, 2017.
16. Theoretical Investigation of Structural, Electronic, and Mechanical Properties of TwoDimensional C, Si, Ge, Sn, , *Crystal Structure Theory and Applications*, 5, 43-55, 2016.
17. Rita John, B. Benita Merlin, Ab Initio Calculations on Structural, Electronic and Optical Properties of ZnO in Wurtzite Phase., John, R. and S. Padmavathi, *Crystal Structure Theory and Applications*, 5(2), 24-41, 2016.
18. S., Umadevi, M., John, R., Lawrence Arockiasamy, A facile synthesis of malic acid capped ZnSe transparent nanopellets and its optical properties, *Sasi Florence, Materials Letters*, 144, 110-113, 2015.
19. Yi Pan, Mohammad A Sohel, Liang Pan, Zengyan Wei, Hanying Bai, Maria C Tamargo, R John, Synthesis of Air-stable PbSe Quantum Dots Using PbCl<sub>2</sub>-oleylamine System, *Materials Today: Proceedings*, 2 (1), 281-286, 2015.
20. S.S., Umadevi, M., Arockiasamy, D.L., John, R., Tailoring of morphology and optical properties of bishydrazone-capped ZnSe nanorods, *Florence Australian Journal of Chemistry*, 68 (10), 1508-1512, 2015.