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### **Publications**

1. D Bharath Raja, K Shanmuga Sundaram, R Vidya, First principle study on hybrid organic-inorganic perovskite  $\text{ASnBr}_3$  (A= Formamidinium, Dimethylammonium and Azetidinium), Solar Energy, Vol.207, Pages: 1348-1355, 2020
2. RM Jebasty, R Vidya, Elucidating reaction equations of  $\text{TiF}_x$  (x= 4, 3, 2) catalysts for hydrogen storage applications, International Journal of Hydrogen Energy, Vol.45 (4), Pages: 2818-2828, 2020
3. PD Sreedevi, R Vidya, P Ravindran, Earth-abundant nontoxic direct band gap semiconductors for photovoltaic applications by ab-initio simulations, Solar Energy, Vol. 190, Pages 350-360, 2019
4. RM Jebasty, R Vidya, Mechanical Properties of Multifunctional  $\text{TiF}_4$  from First-Principles Calculations, ACS Biomaterials Science & Engineering, Vol.5 (4), Pages 2001-2012, 2019
5. T Premkumar, R Vidya, Crystal and electronic structure studies on transparent conducting nitrides  $\text{A}_3\text{N}_2$  (A= Mg, Zn and Sn) and  $\text{Sn}_3\text{N}_4$ , Materials Research Express, Vol.6 (5), Pages:055912, 2019
6. L Patra, R Vidya, H Fjellvåg, P Ravindran, Giant Magnetoelectric Coupling in Multiferroic  $\text{PbTi}_{1-x}\text{V}_x\text{O}_3$  from Density Functional Calculations, ACS omega, 2019
7. PD Sreedevi, P Ravindran, R Vidya, First principles prediction of the ground state crystal structures of antiperovskite compounds  $\text{A}_3\text{PN}$  (A= Be, Mg, Ca, Sr, Ba and Zn), Materials Today: Proceedings, Vol.8, Pages:294-300, 2019
8. RM Jebasty, R Vidya, Calculation of Elastic Properties of Titanium Fluoride Compounds—A DFT Study, International Workshop on the Physics of Semiconductor and Devices, Pages: 1177-1183 ,2017

9. T Premkumar, J Mani, G Anbalagan, R Vidya, Electronic Structure Properties of ATe and A<sub>2</sub>Te (A: Cu, Ag and Cd), International Workshop on the Physics of Semiconductor and Devices, Pages: 1151-1157, 2017
10. R Vidya, G Baskaran, Valence Bond Order and Antiferromagnetism in Silicene-*ab initio* Results, arXiv preprint arXiv:1709.04664, 2017
11. L Patra, MRA Kishore, R Vidya, AO Sjøstad, H Fjellvåg, P Ravindran, Electronic and Magnetic Structures of Hole Doped Trilayer La<sub>4-x</sub>Sr<sub>x</sub>Ni<sub>3</sub>O<sub>8</sub> from First-Principles Calculations, Inorganic chemistry Vol.55 (22), Pages:11898-11907,2016
12. MRA Kishore, H Okamoto, L Patra, R Vidya, AO Sjøstad, H Fjellvåg, P Ravindran, Theoretical and experimental investigation on structural, electronic and magnetic properties of layered Mn<sub>5</sub>O<sub>8</sub>, Physical Chemistry Chemical Physics Vol: 18 (40), Pages: 27885-27896,2016
13. P Manimuthu, R Vidya, P Ravindran, H Fjellvåg, C Venkateswaran, Observation of direct magneto-dielectric behaviour in Lu<sub>3</sub>Fe<sub>5</sub>O<sub>12-δ</sub> above room-temperature, Physical Chemistry Chemical Physics, 2015
14. MF Iozzi, P Vajeeston, R Vidya, P Ravindran, H Fjellvåg, Structural and electronic properties of transparent conducting delafossite: a comparison between the AgBO<sub>2</sub> and CuBO<sub>2</sub> families (B= Al, Ga, In and Sc, Y), RSC Advances, Vol.5, Pages: 1366-1377, 2015

