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Last five years publication list:

- 1. Raja, D.B., Sundaram, K.S. and Vidya, R. First principle study on hybrid organic-inorganic perovskite ASnBr3 (A= Formamidinium, Dimethylammonium and Azetidinium). *Solar Energy*, 207, pp.1348-1355.(2020).
- 2. Jebasty, R.M. and Vidya, R. Elucidating reaction equations of TiFx (x= 4, 3, 2) catalysts for hydrogen storage applications. *International Journal of Hydrogen Energy*, 45(4), pp.2818-2828.(2020).
- 3. Sreedevi, P.D., Vidya, R. and Ravindran, P.,. Earth-abundant nontoxic direct band gap semiconductors for photovoltaic applications by ab-initio simulations. *Solar Energy*, *190*, pp.350-360.(2019).
- 4. Patra, L., Vidya, R., Fjellvåg, H. and Ravindran, P.Giant Magnetoelectric Coupling in Multiferroic PbTi1–x V x O3 from Density Functional Calculations. *ACS omega*, *4*(16), pp.16743-16755.(2019).
- 5. Jebasty, R.M. and Vidya, R.,. Mechanical Properties of Multifunctional TiF4 from First-Principles Calculations. *ACS Biomaterials Science & Engineering*, 5(4), pp.2001-2012.(2019).
- 6. Jebasty, R.M. and Vidya, R., December. Calculation of Elastic Properties of Titanium Fluoride Compounds—A DFT Study. In *International Workshop on the Physics of Semiconductor and Devices* (pp. 1177-1183). Springer, Cham.(2017).
- 7. Premkumar, T., Mani, J., Anbalagan, G. and Vidya, R., 2017, December. Electronic Structure Properties of ATe and A 2 Te (A: Cu, Ag and Cd). In *International Workshop on the Physics of Semiconductor and Devices* (pp. 1151-1157). Springer, Cham.(2017).
- 8. Vidya, R. and Baskaran, G. Valence Bond Order and Antiferromagnetism in Siliceneab initio Results. *arXiv preprint arXiv:1709.04664*.(2017).
- 9. Patra, L., Kishore, M.A., Vidya, R., Sjåstad, A.O., Fjellvåg, H. and Ravindran, P., Electronic and Magnetic Structures of Hole Doped Trilayer La4–x Sr x Ni3O8 from First-Principles Calculations. *Inorganic Chemistry*, *55*(22), pp.11898-11907.(2016).
- 10. Kishore, M.A., Okamoto, H., Patra, L., Vidya, R., Sjåstad, A.O., Fjellvåg, H. and Ravindran, P.,. Theoretical and experimental investigation on structural, electronic and magnetic properties of layered Mn 5 O 8. *Physical Chemistry Chemical Physics*, *18*(40), pp.27885-27896.(2016).
- 11. Manimuthu, P., Vidya, R., Ravindran, P., Fjellvåg, H. and Venkateswaran, C.,. Observation of direct magneto-dielectric behaviour in Lu 3 Fe 5 O 12– δ above room-temperature. *Physical Chemistry Chemical Physics*, *17*(27), pp.17688-17698.(2015)
- 12. Iozzi, M.F., Vajeeston, P., Vidya, R., Ravindran, P. and Fjellvåg, H.,. Structural and electronic properties of transparent conducting delafossite: a comparison between the

AgBO 2 and CuBO 2 families (B= Al, Ga, In and Sc, Y). RSC Advances, 5(2), pp.1366-1377.(2015).