Tata Institute of Fundamental Research
Survey No. 36/P, Gopanpally Village, Serilingampally, Ranga Reddy Dist., Hyderabad - 500107

Seminar

Development and Application of Cutting-Edge Computation in Materials Modelling

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The relevant exploration of novel 2D materials [1, 2] and their applications in catalysis and in next generation *Ultrathin Solar Cell* (Excitonic and Schottky Barrier Solar cell) will be demonstrated. The future prospect of Poisson Boltzmann Solver development in order to treat the solid-liquid interface for such catalytic mechanism would be explained. I would conclude with our recent study on pressure induced Spin-State Transition [3] in connection to our previous investigations on high pressure driven Phase Transformation in super-hard FeB_4 [4] and Thallium [5] with a future outlook about Piezochromism.

References:

1. C. Rupp, S. Chakraborty* et al., ACS Appl. Mater. Interfaces, 8, 1536 (2016)
2. T. Das, S. Chakraborty* et al. J. Mater. Chem. A, to be appeared (2018).
3. H. Banerjee, S. Chakraborty et al, Chemistry of Materials, 27, 5550 (2016).
4. K. Kotmool. T. Kaewmaraya , S. Chakraborty et al., PNAS, 111, 17050 (2014).
5. K. Kotmool. B. Li, S. Chakraborty et al., PNAS, 111, 17050 (2016).

Wednesday, Jan 31st 2018

04:00 PM (Tea/Coffee at 03:30 PM)

Seminar Hall, TIFR-H