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

# Internal Seminar

## A Density Functional Approach on Non-Affine Fluctuations and Stability of Crystal

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We present a theory based on the classical density functional approach, which includes the contributions to the free energy arising due to non-affine displacements to study the freezing of simple liquids in two dimensions. The reduced free energy due to non-affine displacements is given by $h_\chi\chi$, where $h_\chi$ is non-affine field and $\chi$ non-affine parameter. We applied this theory to study the stability of crystal for inverse power potentials (IPP) fluids and Gaussian core model (GCM) fluids and we found that, if non-affine field is negative then it stabilizes the crystal structure. Positive fields have the opposite effect, we also compare our results with simulation data.

***Wednesday, Aug 30th 2017***

***04:00 PM (Tea/Coffee at 03:45 PM)***

***Auditorium, TIFR (FReT-B)***