Tata Institute of Fundamental Research
Survey No. 36/P, Gopanpally Village, Serilingampally, Ranga Reddy Dist., Hyderabad – 500 046

Seminar

Development of Neural Network-based Pauli potential for the Advancement of Orbital-Free Density Functional Theory

Satya S Bulusu

IIT, Indore

For successful implementation of OF-DFT for electronic structure calculations, the Pauli kinetic energy functional and its functional derivative, termed as Pauli potential, play a crucial role. The exact forms of these two quantities are not known. Therefore one employs the approximate forms for the Pauli functional or Pauli potential for performing OF-DFT based calculations. We developed a feed-forward neural network-based representation for the Pauli potential instead of the Pauli functional. Using the neural network-based representation of the Pauli potential, we calculated the ground-state densities of the 1-D model system and for group of atomic systems possessing spherically symmetric ground-state densities.

Wednesday, Nov 27th 2024

16:00 Hrs (Tea / Coffee 15:45 Hrs)

Auditorium, TIFR-H