भारत सरकार /Government of India
परमाणु ऊर्जा विभाग / Department of Atomic Energy
होमी भाभा राष्ट्रीय संस्थान / Homi Bhabha National Institute
राजा रामन्ना प्रगत प्रौद्योगिकी केन्द्र
Raja Ramanna Centre for Advanced Technology

HBNI Faculty Profile

Name	*Arup Banerjee*	
Designation	*Professor*	
Research Area	1. *Concepts of density functional theory and time-dependent DFT for studying properties of many-fermion and many-boson systems.* 2. *Physics and Chemistry of atomic clusters: Electronic, Chemical, and Optical properties of metallic, bi-metallic, and non-metallic clusters.* 3. *Theory of gas adsorption on nano-materials.* 4. *Static and dynamic properties of degenerate properties of Bose and Fermi gases..* 5. *Theory of confined atomic and molecules and neural network based modelling of energy functionals*	
Research Profile	We are engaged in ab initio density functional theory (DFT) and time-dependent DFT (TDDFT) based electronic structure calculations to study various ground state and response properties of several bulk and low-dimensional materials. Neural network based modelling of kinetic and exchange-energy functionals in DFT. Physics and Chemistry of atomic clusters: Electronic, Chemical, and Optical properties of metallic, bi-metallic, and non-metallic clusters. Theory of gas adsorption on nano-materials. Collective oscillations of degenerate Bose and Fermi gases. Theory of confined atomic and molecules. Quantum Optics and Photon-Atom Interaction.	

	Modelling of crystallization process.

Ten Selected Recent Publications

1.	"Generation of atomic-squeezed states in an optical cavity with an injected squezzed vacuum", **Arup Banerjee**, Phys. Rev. A **54**, 5327 (1996).
2.	"Variation-perturbation method in time-dependent density-functional theory", **Arup Banerjee** and M. K. Harbola, Phys. Lett. A **236**, 525 (1997).
3.	"Density-functional theory calculations of total energies, ionization potentials and optical response properties with the van Leeuwen-Baerends potential", **Arup Banerjee** and M. K. Harbola, Phys. Rev. A **60**, 3599 (1999).
4.	"Hydrodynamic approach to time-dependent density functional theory: Response properties of metal clusters". **Arup Banerjee** and M. K. Harbola , J. Chem. Phys. **113**, 5614 (2000).
5.	."Mean excitation energy, static polarizability, and hyperpolarizability of the spherically confined hydrogen atom". **Arup Banerjee** , K. D. Sen, J. Garza and R. Vargas, J. Chem. Phys. **116**, 4054 (2002).
6.	"Calculation of ground- and excited-state energies of confined helium atom", **Arup Banerjee**, C. Kamal and A. Chowdhury, Phys. Lett A **350**, 121 (2006)
7.	"Role of solvent and external growth environments to determine growth morphology of molecular crystals", M. K. Singh and **Arup Banerjee**, Crys. Growth Des. **13**, 2413 (2013).
8.	"Silicene beyond mono-layers - different stacking configurations and their properties", C. Kamal, Aparna Chakrabarti, **Arup Banerjee**, and S. K. Deb, J. Phys. Cond. Mat. **25**, 085508 (2013).
9.	Structural and chemical properties of subnanometer-sized bimetallic Au19Pt cluster, Krishnakanta Mondal, **Arup Banerjee**, and T. K. Ghanty J. Phys. Chem. C **428**, 75 (2014).
10.	Adsorption and Activation of CO2 on Small-Sized Cu–Zr Bimetallic Clusters, Megha, K. Mondal, T. K. Ghanty, and **Arup Banerjee,** J. Phys. Chem. A, 125, 2558, (2021)