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	*Aparna Chakrabarti*	
Designation	*Professor*	
Research Area	*Density Functional Theory; Graphene-like Two-dimensional Materials; Heusler alloys; Transition metal Oxides; Transition metal Chalcogenides*	
Research Profile	*Prof. Chakrabarti has completed her PhD from Indian Institute of Science, Bangalore. After finishing post-doctoral work in University of Arizona, USA, and Fritz-Haber Institute, Germany, she has joined Raja Ramanna Centre for Advancd Technology, Indore as a visiting fellow. She has joined the centre as Scientist E in 2000. She is carrying out studies of geometric, electronic, magnetic and thermoelectric properties of bulk alloys, oxides and hetero- and nano-structures (graphene-like materials) using first-principles calculations. She works in collaboration with experimental and computational material scientists from national and international labs. She has successfully completed an Indo-French and an Indo-German collaborative project.*	

Ten Selected Recent Publications

1.	Bhattacharya, J., Dutt, R. and Chakrabarti, A., Ab-initio predictions of mechanical, electronic, magnetic and transport properties of bulk and heterostructure of a novel Fe-Cr based full Heusler chalcogenide, Journal of Physics & Chemistry of Solids, 178, 111307 (2023).
2.	Bhattacharya, J. and Chakrabarti, A., Electronic and transport properties of Heusler alloy based magnetic tunneling junctions: A first principles study, Computational Materials Science, 216, 111582 (2023).
3.	Baral, M., Srihari, V., Bhakar, A., Chattopadhyay, M. K., Tiwari, P., Chakrabarti, A. and Ganguli, T., Revealing superstructure ordering in Co1+xMnSb Heusler alloys and its effect on structural, magnetic, and electronic properties, Physical Review B 105, 184106 (2022).

4.	Baral, M., Ganguli, T. and Chakrabarti, A., Investigation of structural, magnetic and electronic properties of CoMnSb superstructure: A DFT study, Computational Materials Science, 210, 111441 (2022).
5.	Dutt, R., Bhattacharya, J. and Chakrabarti, A., Investigation of Mechanical, Lattice dynamical, Electronic and Thermoelectric Properties of Half Heusler Chalcogenides: A DFT study, Journal of Physics & Chemistry of Solids, 167, 110704 (2022).
6.	Bhattacharya, J., Pandey, D., Barman, S. R. and Chakrabarti, A., Surface Termination and Thickness Dependent Magnetic Coupling of Cr Adlayers on Ni2MnGa(001) Surfaces: An ab-initio Study, Journal of Magnetism & Magnetic Materials, 540, 168398 (2021).
7.	Gangwar, R., Pandey, D., Kancharlapalli, S., Raychaudhuri, D., Chakrabarti, A., Banerjee, A. and Ghanty, T. K., Ab Initio study of adsorption of fission gas atoms Xe and Kr on MoS2 monolayer functionalized with 3d transition metals, Journal of Physical Chemistry C, 125(2), 1493 (2021).
8.	Dutt, R., Pandey, D. and Chakrabarti, A., Probing the martensite transition and thermoelectric properties of CoxTaZ (Z = Si, Ge, Sn and x = 1, 2): a study based on density functional theory, Journal of Physics: Condensed Matter, 33, 045402 (2020).
9.	Panda, M. R., Gangwar, R., Muthuraj, D., Sau, S., Pandey, D., Banerjee, A., Chakrabarti, A., Sagdeo, A., Weyland, M., Majumder, M., Bao, Q., and Mitra, S., High Performance Lithium-Ion Batteries Using Layered 2H-MoTe2 as Anode, Small, 16(38), 2002669 (2020).
10.	Kamal, C., Pandey, D. and Chakrabarti, A., Isoelectronically substituted group-III based monolayers: An ab initio study, Physical Review B, 102, 085424 (2020).