Functional Materials Design

We have been witnessing a revolution in the innovation of novel functional materials, with discoveries that are important for both fundamental science and industry. The load placed on our environment has grown tremendously in recent years because of the increased consumption of resources and energy, fuelled by entrenched socio-economic activities based on mass production, mass consumption, and mass waste. Under such circumstances, we have to make continuous efforts to develop new materials that tackle global environmental issues such as environmental decontamination, CO₂ reduction, and sustainable resource and energy supply. To address these challenges there is need to pursue both theoretical and experimental R&D approaches. On the theoretical front computational prediction based on first-principles calculations has successfully helped to find an efficient way to develop materials, that demonstrated high efficiency in photovoltaic devices and batteries, promise in single-molecule electronics, high performance ferromagnetic and ferroelectric materials, high-performance thermoelectric materials, and stealth materials for enhanced military capability. In these examples, the first-principles calculations indeed improved the properties of the materials to reach a realistic production level. The computational prowess would not single-handedly help detect the efficient material, but an experimental joint venture is also equally important to test the theoretical outputs. This develop state-of-the-art experimental setups necessitates to with dedicated instrumentation for the synthesis of new functional materials. To meet out these objectives, the Department of Physics in IIT Jodhpur has set up thematic laboratory on Functional Materials Design consisting of dedicated theoretical as well as experimental facilities that can enable the faculty members and students to remain in the forefronts of materials science and engineering.