Press Release

Faculty members of SRM University-AP awarded separate research grants by the National Supercomputing Mission (NSM), Government of India

The project titled "Catalysts for CO_2 Reduction to C_2 Product: Descriptor to Database" has been sanctioned to Prof. Ranjit Thapa, Professor of Physics, SRM University – AP by National Supercomputing Mission (NSM), supported by Department of Science and Technology (DST) in collaboration with the Ministry of Electronics and Information Technology (MeITy), Government of India. The first-year grant of 28 Lakhs of rupees has been received for implementation of the project. Prof. Ranjit Thapa as the project leader has started the work to search the best catalyst to convert CO_2 into useful product and hence solving the problem of climate change due to large production of CO_2 through different sources.

CO$_2$ is a known greenhouse gas and key reason for global warming and climate change. Can we challenge mother nature by converting CO_2, a greenhouse gas into energy with required efficiency? This is a mystery and a mammoth problem and a much-needed problem to be solved with a fundamental approach. Prof Ranjit Thapa believes that metal nano catalyst on support materials can solve the problem and can increase the efficiency of CO_2 reduction to C_2 products, viz., ethylene (C_2H_4) and ethanol (C_2H_5OH). Experimental approach to find the best catalyst for CO_2 reduction needs enormous funds and trials, and a long time is required to develop the exact catalyst for industry application. The mammoth task is to find the suitable composition, shape, and size of metal nanoparticle (MNP) on an appropriate surface for the catalytic reactions. Prof. Ranjit proposes that this can be achieved by computational modelling using Density Functional Theory (DFT) through finding and estimating the electronic descriptor and revealing active sites through structure-activity relations. Recent progress in Machine Learning (ML) for materials with DFT modelling drives towards rational design of catalysts. *The electronic descriptor, storage of MNP/support information in the database followed by prediction using Machine Learning (using predictive model equation) will help to narrow down the search for the best catalyst for CO_2 reduction to C_2 species.*

Dr. Mahesh Kumar Ravva, Assistant Professor of Chemistry, SRM University - AP, received Rs 19.92 Lakhs as the first instalment from DST-National Supercomputing Mission (NSM). The project's main aim is to understand the critical factors that influence the performance of organic solar cells. Using the supercomputer, his research group will model the electronic process that occurs during solar cell operation. The outcome of this project will guide experimentalists to develop organic solar cells with higher efficiency. Organic solar cells are flexible, lightweight, and low-cost and have many exciting applications in wearable electronic devices, smart windows, etc.,

Prof. V.S. Rao, Vice-Chancellor, SRM University – AP and Prof. D. Narayana Rao, Pro Vice Chancellor, SRM University – AP congratulated Prof. Ranjit Thapa and Dr. Mahesh Kumar Ravva.

Prof. Narayana Rao said that necessary facilities and support will be provided by the University to effectively carry out the two projects.