

Report on:
One day Lecture Workshop on “Atomistic Simulation for the Applications of Material Science”

On 6/2/2020, a one-day lecture workshop on ‘Atomistic simulations for the applications of Material Science’ was conducted by the Division of Chemistry of the department of Sciences and Humanities (S&H), Vignan’s Foundation for Science, Technology and Research. The chief guest of the workshop was Dr. D. L. V. K. Prasad, Assistant Professor of Chemistry, IIT Kanpur and the guest of honor for the occasion was Dr. V. Subramanian for CSIR-CLRI, Chennai. The program started with the welcome address by Dr. Srinivasadesikan, convener of this workshop in which he emphasized on the importance of this workshop and stressed that this is the first theoretical chemistry lecture workshop conducted in the university. Dr. K. Prabahakara Rao, the Division Head of Chemistry, explained about the strength of the chemistry division, highlighting the recent achievements of the division. Prof N. Srinivasu, HoD, S&H pointed out the highlights of S&H department and also stressed about the utility of theoretical chemistry in today’s world. Both the guests have expressed their views on the importance of such kind of workshop emphasizing the long-term goals of implementing theoretical concepts in physics and chemistry to modern-day research.



In the opening lecture, Prof. V. Subramanian, The Chief Scientist, CSIR-CLRI, Chennai started his talk with the historical development of computational chemistry and he explained the importance of molecular modeling for various applications in chemistry and biology.



He highlighted various interactions between alpha helix of protein and the different configurations of graphene through molecular simulation. He also highlighted the effects of dopants onto the graphene surface especially with silicon and their subsequent influence on protein folding.



Dr. D. L. V. K. Prasad, IIT, Kanpur started with the basics of quantum mechanics including Schrodinger equation. He delivered his talks highlighting the milestones of computational chemistry for materials and also provided a glimpse of his past and present research works. His interactive teaching style, and exceptional oratory skills made the session very exciting and enjoyable.

In the valedictory program, all the dignitaries congratulated the convener, the organizing committee, the research scholars for making this program a successful one.