



ST. XAVIER'S COLLEGE, MAPUSA GOA

College with Potential for Excellence
Re accredited by NAAC with A Grade
Awarded DBT STAR College Scheme

Nature of Event (Workshop, Guest Lecture, Addon Course, Seminar, etc.)	Hands-on session (Workshop)
Name of Department	Chemistry
Faculty In-charge	Dr. Johnross V. Albuquerque
Stratum of Event (College, State, Regional, National)	College
Title of Event	Computational Chemistry
Date of Event	11 th January 2023
Venue	Computer Lab, Post Graduation Block, St. Xavier's College, Mapusa-Goa
Resource Person details	Prof. Rajendra Shirsat Professor in Physical Chemistry, School of Chemical Sciences, Goa
Objective/ Scope of Event	To provide the participants an opportunity to learn the subject of Computational Chemistry by providing them hands-on training on how to use MS Excel in Chemistry.
Particulars of Event	Computational Chemistry is a subject where Chemistry can be studied with the aid of computers. The resource person Prof. Shirsat introduced the subject for about 1 hour before engaging the participants with MS Excel exercises. Participants mostly MSc. Part II students and faculty members learnt how to plot molecules in MS Excel using cartesian coordinates and how MS Excel would give bond lengths/bond angles. Huckel Theory and its applications were discussed and plotting of orbitals.
Outcome of Event	Participants learnt how to use MS Excel to view planar molecules, calculate bond lengths/ bond angles and several other Excel features.
Feedback	Very informative and interesting

Total No. of Participants

18 post graduate students and 4 faculty members

Photographs

