



**Workshop on**  
**Introduction to Gaussian & Drug Discovery**  
**Theory & Practice**

Venue: Department of Chemistry, BUET  
<http://chem.buet.ac.bd/workshop-2020/>

**15<sup>th</sup>**  
**Feb 2020**  
**Saturday**

Time	Topics	Instructors
<b>8.30-9.00 AM</b>	Registration	
<b>9.00-9.05 AM</b>	Inauguration	<b>Dr. Md. Shakhawat Hossain Firoz</b>
<b>9.05-9.10 AM</b>	Introductory speech by special guest	<b>Prof. Dr. Md. Saiful Islam</b> IICT, BUET
<b>9.10-9.30 AM</b>	Introduction to Computational Chemistry <ul style="list-style-type: none"> <li>a. What is computational Chemistry?</li> <li>b. Background</li> <li>c. List of computational software</li> <li>d. Gaussian Software</li> <li>e. Gaussian Methods</li> <li>f. Applications and Significance</li> <li>e. Tools</li> </ul>	<b>Dr. Abu Bin Imran</b>
<b>9.30-10.00 AM</b>	Introduction to Gaussian & Gauss View software <ul style="list-style-type: none"> <li>a. DFT, b. BASIS Set, c. Tools</li> </ul>	<b>Mohammad Mazharol Haque</b>
<b>10.00-10.15 AM</b>	Tea Break	
<b>10.15 -1.00 PM</b>	Hand on Session <ul style="list-style-type: none"> <li>a. Build a Molecule</li> <li>b. Job Submit</li> <li>c. Output file</li> </ul>	<b>Ajoy Kumer &amp; Ashutosh Nath</b>
<b>1.00-2.00 PM</b>	Lunch Break	
<b>2.00-2.20 PM</b>	Oral session on Chemical reactivity <ul style="list-style-type: none"> <li>a) HOMO, LUMO</li> <li>b) IP, EA, softness, hardness, chemical potential etc.</li> <li>c) Thermo-dynamical evidence</li> <li>d) ESP and PES</li> </ul>	<b>Ajoy Kumer</b>

<b>2.20-4.00 PM</b>	Hand on Session d. IR, UV, NMR h. HUMO, LUMO h. S <sub>N</sub> 2 Reaction Mechanism i. ESP, PES	<b>Mohammad Mazharol Haque</b>
<b>4.00-4.15 PM</b>	Tea Break	
<b>4.15-6.00 PM</b>	Drug Discover a. Introduction to Docking b. Docking Tools i. PyMol ii. PyRx iii. Discover Studio	<b>Ajoy Kumer &amp; Ashutosh Nath</b>
<b>6.00-6.15 PM</b>	Certificate giving and Closing Session	<b>Dr. Md. Shakhawat Hossain Firoz</b>