

**Computational Chemistry Workshop for Students of the
School of Science and Engineering
Yvonne A. Ewell Townview Magnet Center
Dallas, TX 75203
Organized by CATCO at SMU
Fondren Science Building, Department of Chemistry
Saturday, August 20, 9 am to 6 pm**

9:00 to 9:15 am	Welcome; getting name tags; presentation of CATCO members
9:15 to 9:30 am	Introduction to Computational Chemistry, Dieter Cremer
9:30 to 10:30 am	<i>Unit 1:</i> Quantum chemical description of the water molecule (molecular properties,; what is a H-bond; liquid water; H-bonding in biomolecules) Elfi Kraka
10:30 to 10:45 am	Break
10:45 to 11.45 am	<i>Unit 2:</i> Quantum chemical description of benzene (pi-delocalization as a genuine quantum chemical effect; pi-bonding; metallic bonding; ferrocene) Dieter Cremer
11:45 to 1:00 pm	Lunch break; during lunch possibility of asking questions about SMU, Department of Chemistry, studying Chemistry; job situation; etc.
1:00 to 2:00 pm	<i>Unit 3:</i> Quantum chemical description of fullerenes (allotropic forms of carbon; properties of C60; frontier orbital pictures, superconductivity) Dieter Cremer
2:00 to 2:15 pm	Break
2:15 to 3:15 pm	<i>Unit 4:</i> Molecular modeling of surfactants Rob Kalescky
3:15 to 4:15 pm	<i>Unit 5:</i> Docking of a drug into a protein (molecular modelling; key-lock principle; molecular mechanics) Marissa Tyro
4:15 to 4:30 pm	Break
4:30 to 5:30 pm	<i>Unit 6:</i> Quantum chemical investigation of chemical reactions (PES, reaction path, transition state, activation energy and reaction enthalpy) Elfi Kraka
5:30 to 6:00 pm 6:00 pm	Campus walk; SMU history; how is it to be a student at SMU Farewell