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[[Home](#)] [[Moodle](#)]

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Molecular Modeling and Chemical Information

Fall 2016

Instructors: Carl Dirk and James Salvador

Molecular Modeling assignments will be provided by Dr. Dirk through Blackboard and must be submitted through email to cdirk at utep dot edu.

Chemical Information and Programming assignments must be submitted through the course Moodle.

Week	Date	Molecular Modeling	Chemical Information	Programming
1	August 26	Introduction in LART 403		
2	September 2		Logins	Downloading and installing the required software. (4:48) Introduction to Linear Programming. (12:07) Introduction to Visual Programming. (16:17) Introduction to Event Programming. (10:38) First Challenge Exercise: A Simple calculator. (8:08)
3	9			Introduction to Java Bean Components. (6:16) Introduction to Drawing. (10:18) Introduction to Event Driven Drawing. (10:04) Introduction to Lists. (12:22) Second Challenge Exercise (8:19)
4	16		Namesake Text Search	Introduction to Datatypes. (16:43) Introduction to Translation or Move. (11:36) Preparing for Rotation. (13:42) Introduction to Rotation. (8:34) Third Challenge Exercise: Changing Modes (5:48)
				Introduction to Rolling. (10:42)

5	23			Introduction to Scaling. (5:50) Introduction to Centering. (8:31) Introduction to Fit. (7:50) Fourth Challenge Exercise: New... (3:47)
6	30			Introduction to removing event methods. (5:08) Introduction to the electron and extensions. (6:20) Introduction to properties and methods of atoms and electrons. (4:41) Introduction to stitching the atoms and electrons. (11:28) Introduction to drawing the bonds. (7:17) Fifth Challenge Exercise: Generalizing methods (3:47)
7	October 7	Follow the updated syllabus emailed to you by Dr. Dirk	Video instructions through Blackboard	Introduction to Libraries. (18:05) Introduction to Displaying Information (7:44) Introduction to whichAtom (17:49) Implementing whichAtom (11:27) Sixth Challenge Exercise: Fixing Problems with if (2:19)
8	14	Email your completed homework to		Introduction to Re-Centering (2:44) Introduction to Z Sorting (14:56) Preparing the Periodic Table (7:33) Seventh Challenge Exercise: Periodic Table (14:27)
9	21			Introduction to the Optimization Problem (10:25) Introduction to Numerical Analysis: Newton Raphson (13:25) Application of Newton-Raphson to Optimization (9:29) Implementing Optimization (19:30) Eighth Challenge Exercise: New Again (4:02)
10	28			Introduction to Thread Programming (9:56) Introduction to Auto Stop (8:06) Introduction to Writing Files (17:16) Introduction to Reading Files (13:39) Ninth Challenge Exercise: Random (2:23)
11	November 4			Introduction to drawing polygons. (11:42) Introduction to lighting. (17:39) Introduction to a parametric plotter. (13:13) Implementing arch bonds. (20:48) Tenth Challenge Exercise: Light (1:10)
12	11			Introduction to hemispheres. (12:52) Fixing the arches. (5:17) Introduction to perspective. (9:37) Fixing perspective input. (9:10)

			Reference Management	Eleventh Challenge Exercise: Parallax (5:32)
13	18			Moving One Atom. (9:46) Rotate and Roll Around an Atom. (10:07) Manipulation of one molecule. (21:57) Twist. (16:42) Twelfth Challenge Exercise: Templates (10:10)

After being graded, 5 % per day will be deducted for late submissions. For example, if your work earned a 90 % but you turned it in 2 days late, then your grade for that assignment will be 80 %.

All molecular modeling, chemical information, and programming assignments will be weighted equally.

Your assignment grades will be averaged to give your course grade as follows: A > 89.5 %, B > 79.5 %, C > 69.5 %, D > 59.5 %.

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Office Hours: MWF 8:30-9:30 am, TR 9 to 10:30 am or by appointment.