10.491 Integrated Chemical Engineering Spring 1999

Material Property Estimation and Design

Instructor: Gregory C. Rutledge
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Teaching Assistant: Numan Waheed
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Meeting times: MTWF 10-11am, 66-144

Office hours: M 1-2pm (Rutledge)
Th 4-6pm (Waheed)

Recommended texts: Web Site: http://heavenly.mit.edu/~eprof

Van Krevelin, Properties of Polymers, 3rd ed., Elsevier: Amsterdam, 1990.

Rowley, R.L., Statistical Mechanics for Thermophysical Property Calculations, Prentice Hall: Engelwood Cliffs, NJ, 1994.

Billmeyer, F.W., Textbook of Polymer Science, 3rd ed., Wiley Interscience: New York, 1984.

Grading:		
	homework sets	50%
	design project	40%
	class participation	10%
	(no final exam)	

This module is a case study of a product design problem, with a focus on development of an environmentally benign new polymer. We will look at the influence of molecular structure on properties of polymers and learn to use state-of-the-art computer simulations to characterize polymers and generate estimates of material properties.

Most assignments will make use of the MSI suite of molecular simulation modules, accessible from any Athena SGI workstation, as well as from SGI workstations in the department graphical workstation cluster located in 66-008.

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Module III: Material Property Estimation and Design April 7 - May 12

	Date	Topic	Reading assignment
Week 1	Apr. 7,9	Issues and Methods in Product Design	Narayan Hocking Reid et al
Week 2	Apr. 12 Apr. 13,14,16	*Electronic classroom session, 4-035* Introduction to Polymer Properties	 Web pages: Introduction to Polymers, conformation, tacticity
Week 3	Apr. 19,20 Apr. 21,23 Apr. 21	Patriots' Day Holiday Methods for Estimating Properties of Materials *Electronic classroom session, 4-035 (4-6pm)*	 Group contributions Topology method
Week 4	Apr. 26 Apr. 27,28 Apr. 30	*Electronic classroom session, 4-035* Methods for Estimating Properties of Materials (cont) *No class*	 Molecular simulation
Week 5	May 3 May 4,5,7	*Electronic classroom session, 4-035* Product Design Considerations	 Engelberg and Kohn Gilbert et al Outside reading
Week 6	May 10 May 11,12	*Electronic classroom session, 4-035* Design presentations	

Notes:
1. Each Monday with the exception of Patriots Day (Apr. 12, 25, May 3,10) the class will meet in the Athena cluster in Room 4-035 for a computational laboratory in molecular simulation.

2. There will be no class on Friday, Apr. 30. Instead, we will have a special evening electronic classroom session from 4-6pm on Apr. 21.