VCU Discrete Mathematics Seminar

A graph theoretic model to explain 'what every chemist knows'

Craig Larson
VCU!

Tuesday, Dec. 3
12:30–1:20
4119 Harris Hall

ABSTRACT: We discuss the use of graph theory in representing molecular structure, gently introduce the calculation of the determinant of a graph, and then propose a simplified Hückel-type molecular-orbital (MO) model for the valence electrons of saturated hydrocarbons and consider the consequent eigenvalue spectrum. We obtain a first foundational result, which every chemist "knows", namely that: alkanes are stable, with half their (Hückel-type MO) eigenvalues positive and half negative. We leave open the conjecture that this is also true for the full class of saturated hydrocarbons with a specific interaction constant. This is joint work with Doug Klein.

For the full schedule of speakers, titles and abstracts for Fall 2013, see:
`http://www.people.vcu.edu/~dcranston/DM-seminar/`