The Long Island Subsection
Of the New York American Chemical Society

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A seminar by:

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Title of Talk: "Guided inquiry in organic chemistry: Using computational methods to introduce molecule building and geometry."

Synopsis: We developed a guided-inquiry computational activity for sophomore Organic Chemistry, in which students use the Gaussian program to perform simple quantum mechanical calculations to discover the connection between atomic interactions, steric hindrance and isomerism. The activity contains a series of steps for constructing organic molecules, calculating bond angles and lengths, and analyzing the nuclear repulsion and total potential energy of the structures. This process lets students discover the energetic differences between cis and trans isomers of small alkenes. The exercise precedes the lecture introduction of isomers and allows students to build their own understanding of steric hindrance. The traditional lecture is then used to review the concept of isomerism and solve problems to further strengthen student understanding. One of the most essential goals of the exercise to reinforce key concepts of atomic structure and nuclear interactions that govern molecular conformations. Summary questions are included at the end of the activity to emphasize these concepts. Short anonymous surveys were distributed to the class upon completion of the activity, and the feedback that was obtained from the students was overwhelmingly positive. This activity can easily be adopted into any Organic Chemistry I curriculum, and can be modified to fit other software programs.

All are welcome!

When: Thursday, April 19th, 2018
***Where*:** Queensborough Community College, Science Building Rm S-112
Time: 5:30 p.m. – Social w/ Light Refreshments; 6:00 pm – Seminar Start
Directions: http://www.qcc.cuny.edu/about/driving.html
After Seminar Dinner: At a nearby restaurant, $25 per person.