

HW # 4. Assigned 9/18, due 9/24.

1. Consider treating polyenes, ethylene, butadiene, hexatriene, etc., with the one-dimensional particle-in-the-box model. What length polyene (i.e., number of C atoms) is required to absorb light in the red region of the spectrum? How does that compare with the conjugated portion of carotene?
2. Again using the particle-in-the-box problem, predict in eV the first IP and electron affinity of hexatriene. What temperature would be needed to achieve 10% population of the normally lowest unoccupied molecular orbital (LUMO)?
3. Consider an electron in one, two, and three dimensional boxes with a side of 4 Å. How does the zero-point energy vary with increasing dimension?