

Selected Answers

The work that I received was excellent. A couple of additional points...

Points of emphasis:

- EDG generally raise HOMO energy because the HOMO is an *antibonding* combination of the C=C π orbital and the EDG π or lone pair orbital
- EWG generally lower LUMO energy because the LUMO is a *bonding* combination of the C=C π^* orbital and the EDG π^*
- Don't get misled by an MO's delocalized shape. When you look at MO surfaces, different "balloons" may look like parts of a Lewis structure, e.g., a π bond or a lone pair, but the correct ways to think about the MO are:
 - I can see how the MO came to be: it combines localized pieces
 - I can see what the electrons in the MO do for the molecule: they change its energy by creating some bonding here and some antibonding over there, and they change its polarity by loading some atoms up with negative charge while depriving others

Point of correction:

- As the following images show (HF/3-21G model), the HOMO of nitroethylene is not located on the C=C group at all. You should use HOMO-1 (and LUMO) to estimate the electron withdrawing effect of NO₂ on the vinyl group. (**Note on perspective:** These are the 5 low energy "valence" π MOs. Therefore, these orbitals have a node in the molecular plane and there are two lobes, in front and behind the molecular plane, of opposite sign. Since we are viewing the MOs from a direction perpendicular to the molecular plane, the front lobe perfectly hides the back lobe.)

