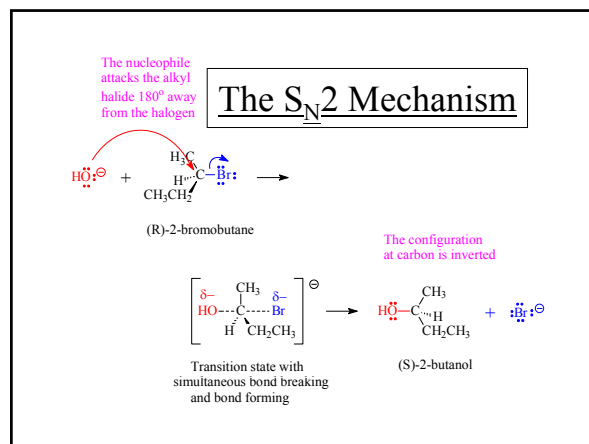


We can use bonding theories to explain reactions and reactivity

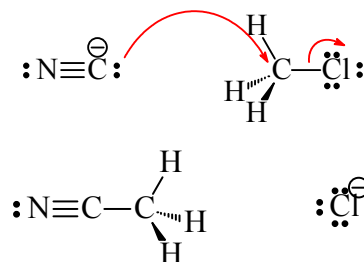
- **Lewis structures** allow us to “push electrons” but explain little
- **Valence bond theory** allows us to use Lewis structures in a natural way, bringing in “resonance,” “hybridization” and “orbital overlap.”
- **Molecular orbital theory** allows us to explain how bonds are formed and broken by donation of electrons from a HOMO to a LUMO



How do we explain this?

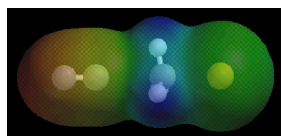
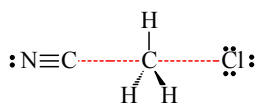
- Lewis/Valence-bond theory does not allow an explanation but does allow us to “push the electrons” to provide a [convenient picture](#).
- “Frontier MO theory” allows us to explain this in terms of the donation of electrons from the HOMO of the nucleophile to the LUMO of the alkyl halide electrophile.

Molecular orbitals: Lewis picture of the S_N2 reaction

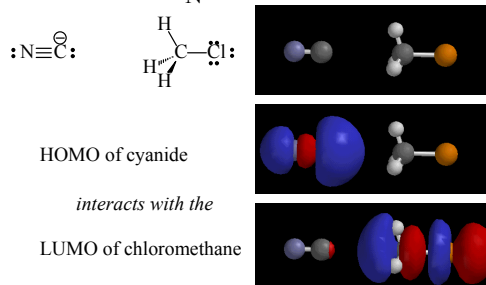


Transition state for the S_N2 reaction can be explained with valence-bond theory

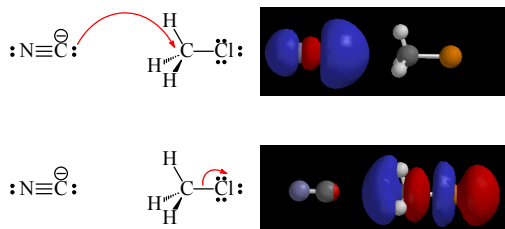
- Bond to chlorine breaks as the bond to cyanide forms.
- Notice that **negative charge** is spread “evenly” between the nucleophile and the leaving group.
- **But why must attack be from the backside?**



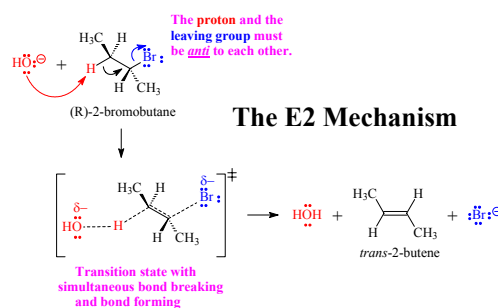
Frontier molecular orbitals in the S_N2 reaction



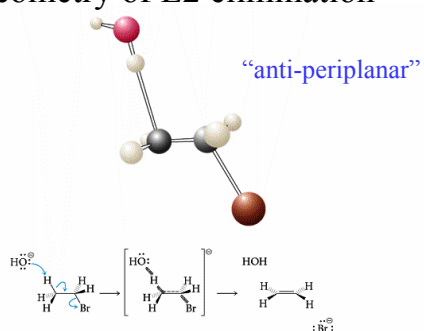
Molecular orbitals are required to explain backside attack!



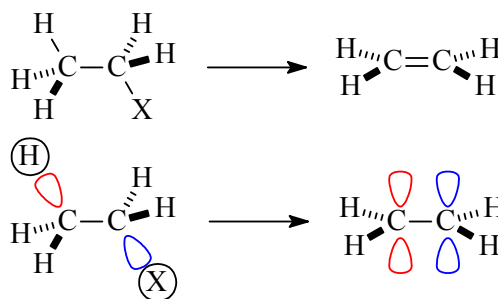
The proton and the leaving group must be anti to each other.



Geometry of E2 elimination



Geometry of E2 elimination



Geometry of E2 elimination:
Frontier Molecular Orbitals

