

Manual PES at static locators for PD

Correlate HF MOs to SAPT energy.

Combine Cation + Anion - Cancelling each other out

Add lithium - most extreme HOMO raising
- most extreme HOMO/LUMO lowering

Jeffrey Reimers

"Virial theorem"

$$R_2 \rightarrow T \geq -\frac{1}{2} V$$

