Valence-hole electron configurations: A new global electronic structure paradigm for C_2 (and possibly beyond)

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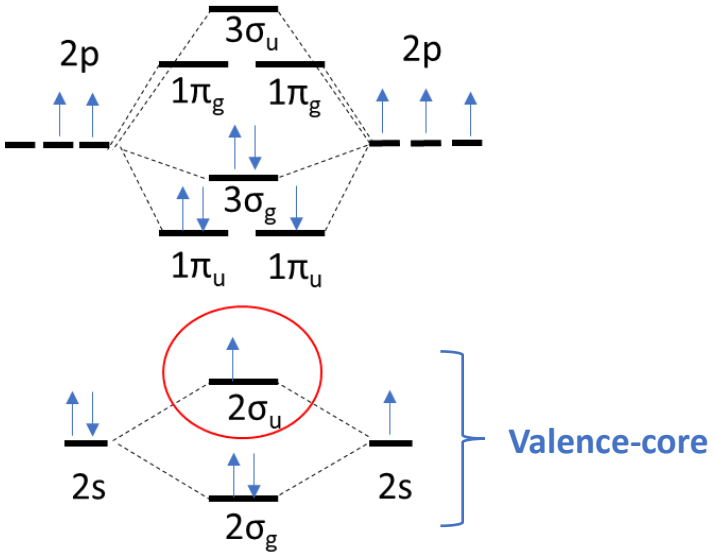
Chemical intuition!!!

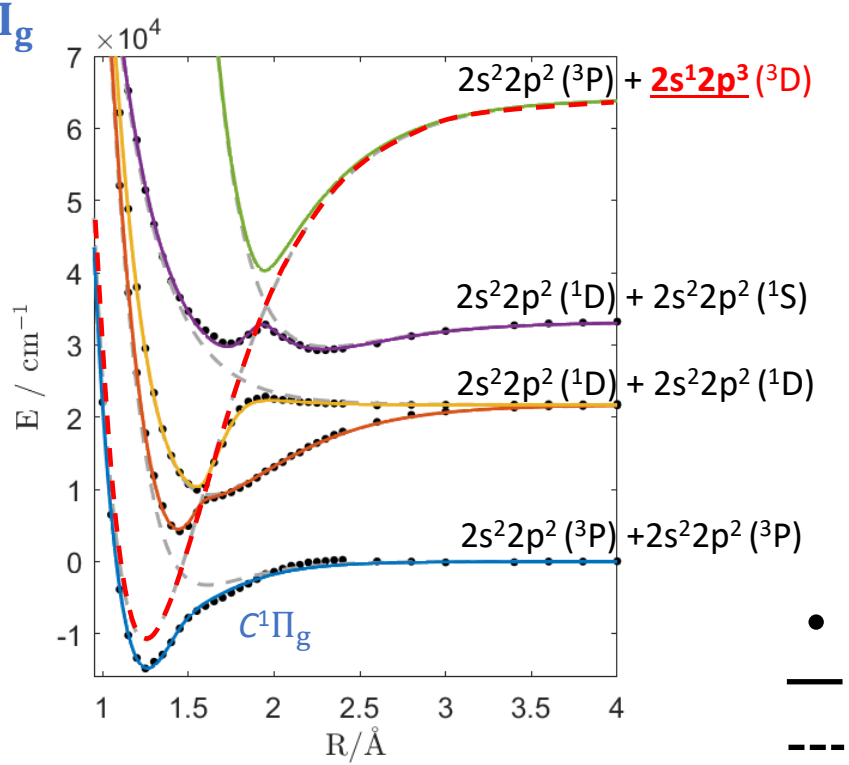
Valence-hole state:
$3\sigma_g/1\pi_u \leftarrow 2\sigma_u$

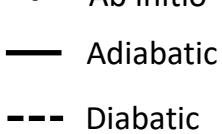
- Nominal bond order of 3
- At large R, correlates to $2s^22p^2$+**$2s^12p^3$**



- The electronic structures of low-lying $^1\Pi_g$ and $^3\Pi_g$ states are systematically disrupted due to curve-crossings with the deeply-bound, valence-hole states
- The effects of the valence-hole-induced curve-crossings are gloriously sampled in the molecular constants derived from the laboratory spectra of C_2

$^1\Pi_g$





$^3\Pi_g$