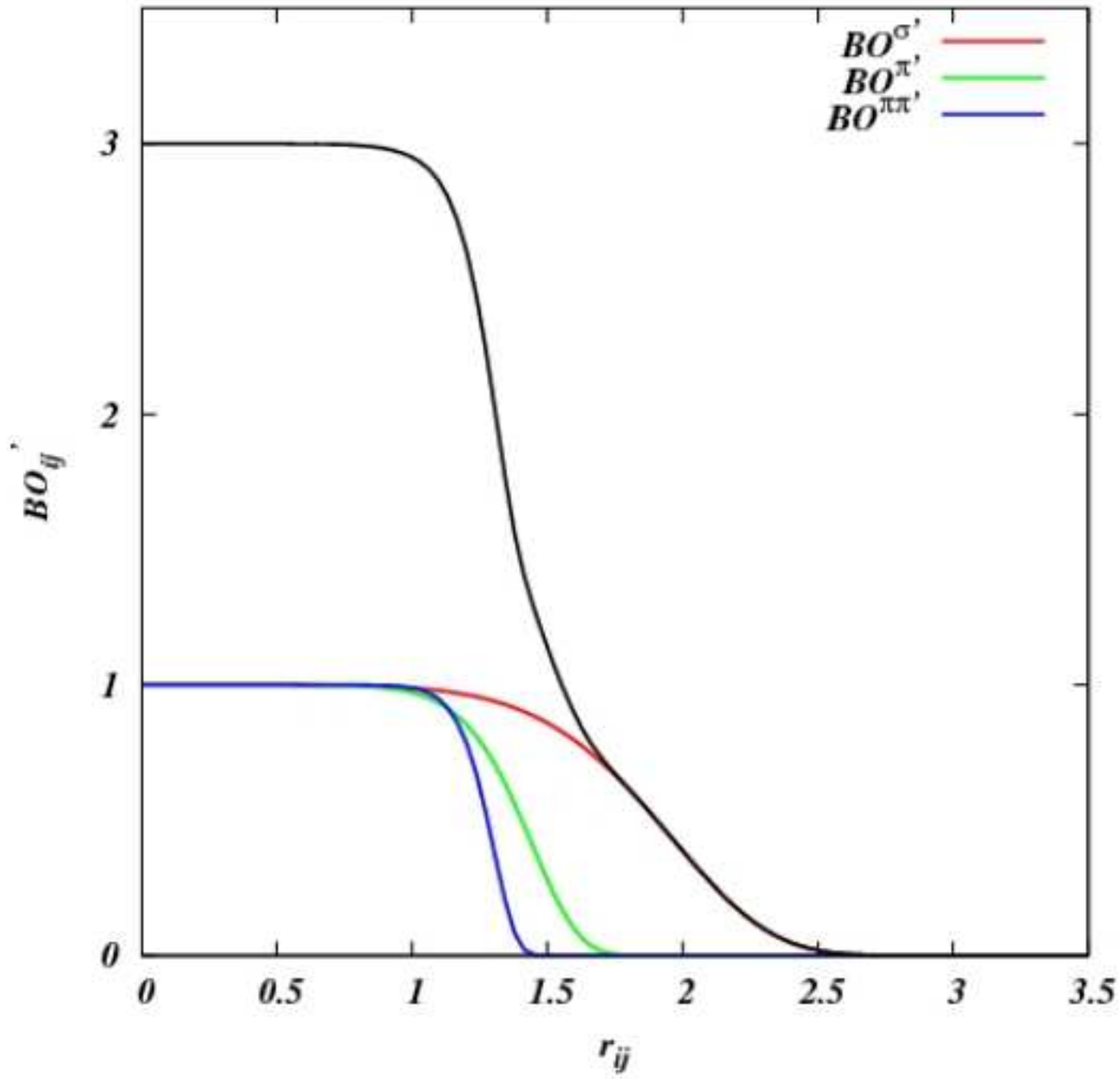
- Uncorrected bond order:

$$BO_{ij}^{\alpha'}(r_{ij}) = \exp\left[a_\alpha \left(\frac{r_{ij}}{r_{0_\alpha}}\right)^{b_\alpha}\right]$$

Where α is for
σ–σ, π–σ, and π–π bonds

- The total uncorrected bond order is sum of three types of bonds
- Bond order requires correction to account for the correct valency



Bond order for C-C bond