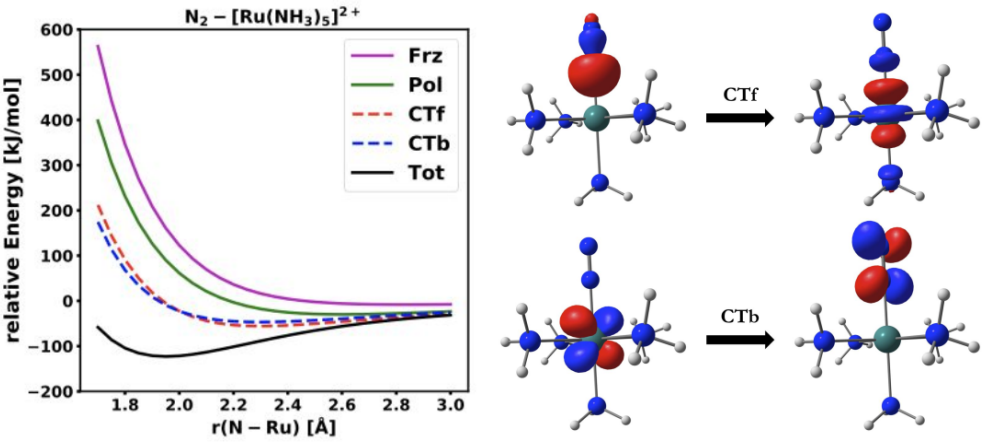
Q-CHEM™
A Quantum Leap Into the Future of Chemistry

Analyzing the Effect of Charge Transfer Using Absolutely Localized Molecular Orbitals



- Charge transfer (CT) in ALMO-EDA: stabilization effect due to inter-fragment orbital relaxation;
- Perturbative charge-transfer analysis (CTA): decomposition of the amount of CT (ΔQ) and the associated energetic stabilization (ΔE) into forward and backward contributions;
- Complementary occupied/virtual pairs (COVP) analysis:
  - Based on perturbative CTA;
  - Rotates the polarized ALMOs within a molecule to achieve a compact orbital representation of CT between a pair of molecules;
  - Helps chemists quantify and visualize CT effects.
- Variational forward-backward (VFB) analysis:
  - Decomposes CT stabilization energy into forward and backward contributions using two variationally optimized "one-way" CT states;
  - Can be seamlessly integrated with the adiabatic ALMO-EDA scheme, facilitating analysis of the effects of forward and backward CT on molecular properties.

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