Out of equilibrium electronic distribution topological descriptions. The simple atomic B3+ cluster case

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Abstract

The local and non-local topological treatment of electronic distributions is applied to a simple out of equilibrium case of a three-atom cluster. The bending movement of evolution is described in detail through the onset and disappearance of critical points defining two kinds of molecular structures, each of them containing an equilibrium geometry and also describing a transition state (TS). A structural change is also found and analyzed through the behavior of population magnitudes from the paired and unpaired electron densities. All points in this rich evolution are featured and distinguished by the mentioned local and non-local magnitudes. Furthermore, the multi-center bonding interactions are discussed in this context to give a complete description of the changes undergone. Consideration of the electron correlation effects constitutes the basement of the results gathered, thus showing their main influence in breaking and making boron bonding interactions.

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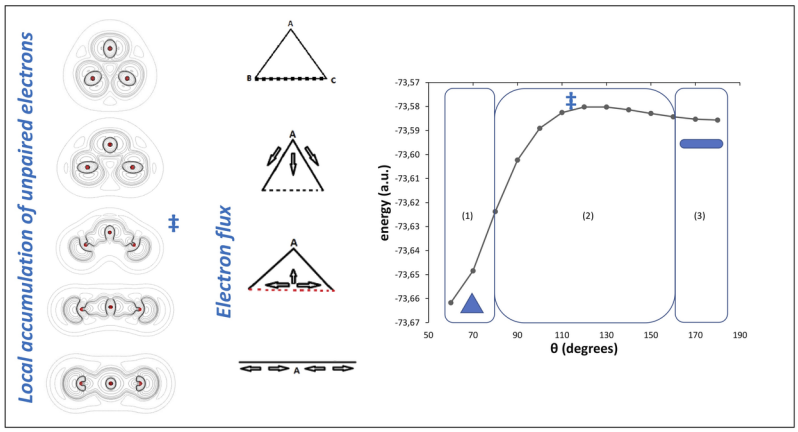

Figure 1: Laplacian contour maps of effectively unpaired densities for **equilibrium I** ($\vartheta = 600$), $\vartheta = 800$; **transition state (TS)** ($\vartheta = 125.70$); $\vartheta = 170.000$, and **equilibrium II** geometries; graphical representation of the system (line with squares indicates the distance that increases sequentially); schemes of charge flux corresponding to regions (1), (2) and (3), ring configuration, transition (TS) and linear configurations stages respectively and energy values (Hartrees) as a function of the sequential changes of the control parameter (angle BAC in degrees, ϑ).