Molecular forces reveal molecular reactivity

Piotr Ordon

Wrocław University of Environmental and Life Sciences, 25 Norwida St., 50-375 Wrocław, Poland

1. We derived the procedure that deliver the mechanism of the chemical reaction from the atomic divergences of the Hellmann – Feynman forces. We have identified special critical points on the reaction path where chemical bonds are being broken and formed. This way we reveal the sequence of events along the reaction path that constitute a coherent description of the reaction mechanism.

2. With the use of the atomic divergence of Hellmann – Feynman forces and Feynman electrostatic theorem, we derived the new gradient theorem that links linear response function and reactivity indices directly to the electron density gradient. This theorem is a source of the new expressions for the reactivity indices which are derivatives of the electron density. This way we have obtained the Fukui Function index, local softness as well as the higher derivatives of electron density.