

On the Electrical analogy of the Condensed Linear Response function from CDFT

GRINCOURT Rémi; HOFFMANN Guillaume; CHERMETTE Henry; MORELL Christophe

Institute of Analytical Science UMR 5280, University of Lyon 1 (Claude Bernard), 5 rue de la Doua 69100 Villeurbanne, France

remi.grincourt@ens-lyon.fr

Within this poster presentation, the diagonalized element from the Condensed Linear Response function stemming from conceptual density functional theory (CDFT)¹ will be discussed. Mainly, using the definition of the Condensed Linear Response function² ($\chi(r, r')$), on the relationship between the variation in electron density and the variation in external potential leads us to propose an analogy with a capacitor. This analogy will be presented on several molecules (such as H₂, HCN, HCCH, ...) where the results appears promising. And leads us to a better understanding of the linear response function and, therefore, chemical reactivity³.

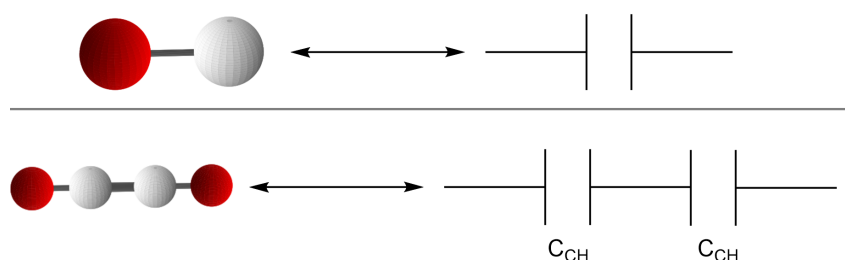


Figure 1: On top, the schematic representation of the first eigenvector of the Linear Response function for H₂. This eigenvector is analogous to a single capacitor. On the lower part, the schematic representation of the second eigenvector of the Linear Response function for acetylene (HCCH). This eigenvector is analogous to two capacitor in series.

Keywords: Conceptual DFT; Condensed Linear Response function; Capacitance

¹Chermette, H., Chemical reactivity indexes in density functional theory. *J. Comput. Chem.*, 1999, 20, 129-154.

²Geerlings, P. et al. Conceptual DFT: chemistry from the linear response function, *Chem. Soc. Rev.*, 2014, 43, 4989

³Guégan, F., Abid-Charef, Y., Hoffmann, G. et al. Finishing (off) the Klopman–Salem model: the importance of density polarization energy. *Theor. Chem. Acc.*, 2023, 142, 104