

Chemical reactivity from linear response eigenfunctions and eigenvalues

Rémi Grincourt,^a Guillaume Hoffmann,^a Frédéric Guégan,^b Vincent Tognetti,^c Laurent Joubert,^c Henry Chermette,^a Alejandro Toro-Labbé,^d and Christophe Morell^a

^a Université Claude Bernard Lyon 1, UMR 5280 CNRS, 5 rue de la Doua, 69100 Villeurbanne, France

^b 2IC2MP UMR7285 Université de Poitiers, Poitiers, France

^c Institut CARMEN UMR6064(ex lab. COBRA), Université de Rouen, INSA Rouen, CNRS, 1 Rue Tesnière, Mont-Saint-Aignan, 76821 Cedex, France

^d Laboratorio de Química Teórica Computacional (QTC), Facultad de Química y de Farmacia, Pontificia Universidad Católica de Chile, Chile

E-mail address: Christophe.morell@univ-lyon1.fr

The Static Linear Response Response Function is a six dimension kernel that gives the evolution of the electron density in a location $\mathbf{r}$ when the external potential is modified in a position $\mathbf{r}'$. This kernel can be diagonalized, and the associated eigenvectors thus obtained form a complete basis set on which any density deformation can be projected on. In this presentation, we propose to interpret these vectors as Electron Density Deformation Modes (EDDM). Each eigenvector represents a mode describing how electron density is modified in response to an external potential perturbation. It is hypothesized that these modes can reveal the preferred direction or pattern of electron flow, helping identifying the reactive region of a molecule.

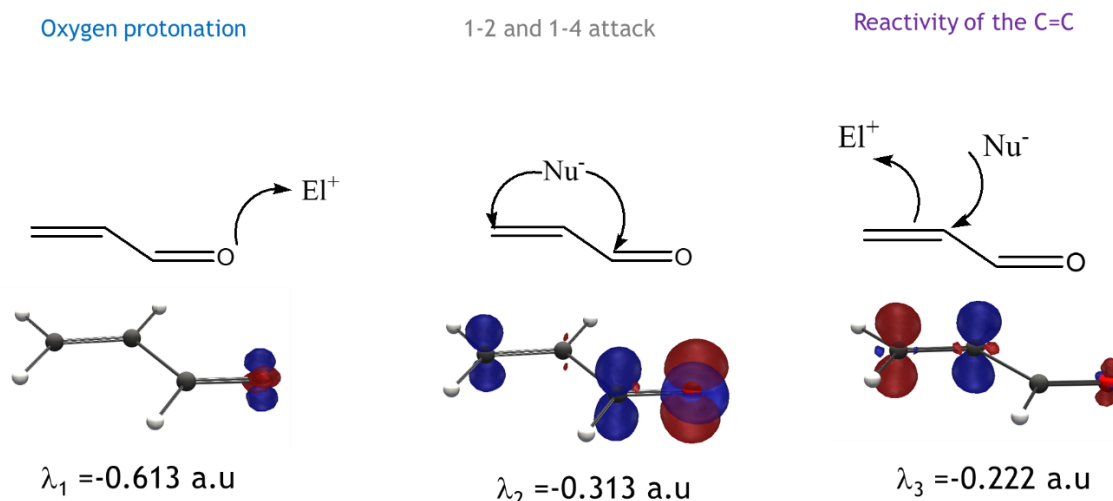


Figure 1. First three eigenvectors and eigenvalues of acrolein.

References

1. R. Grincourt, G. Hoffmann, F. Guégan, V. Tognetti, L. Joubert, H. Chermette, A. Toro-Labbé, C. Morell; Chemical reactivity from linear response eigenfunctions and eigenvalues. *J. Chem. Phys.* **2025** 163 (13), 134118.