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"THE BASIS ELECTRONIC ACTIVITY OF CHEMICAL SYSTEMS. A THEORY OF BOND REACTIVITY"

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We present the Basis Electronic Activity (BEA) of molecular systems, it corresponds to the significant, although non-reactive, vibrationally induced electronic activity that takes place in any molecular system. Although the molecule's BEA is composed by equal number of local contributions as the vibrational degrees of freedom, our results indicate that only stretching modes contribute to it. To account for this electronic activity, a new descriptor, the Bond Electronic Flux (BEF), is introduced. The BEF combined with the force constant of the potential well hosting the electronic activity give rise to the Effective Bond Reactivity index (EBR), that turns out to be the first DFT-based descriptor that simultaneously accounts for structural and electronic effects. Besides quantifying the bond reactivity, EBR provides a basis to compare the reactivities of bonds inserted in different chemical environments and paves the way to exert selective control to enhance or inhibit their reactivities. The new concepts formulated here, and the associated computational tools, are illustrated with the characterization of the BEA of a set of representative molecules. In all cases the BEFs follow a linear pattern whose slopes indicate the intensity of the electronic activity and quantify the reactivity of chemical bonds.

References

[1] Benítez, F.J.; Gutiérrez-Oliva, S.; Herrera, B. and Toro-Labbé, A: The Basis Electronic Activity of Chemical Systems. A Theory of Bond Reactivity, *J. Phys. Chem. A* 2024, in press. (https://doi.org/10.1021/acs.jpca.4c00359)