

# ELF<sup>&</sup>IGM: A Modern Take on Electron Localization Function Topological Analysis

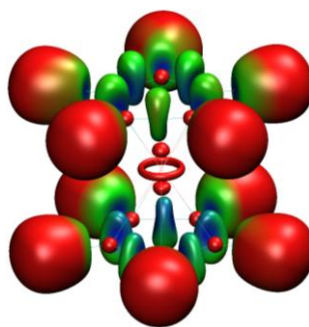
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The Electron Localization Function <sup>1</sup> (ELF) has been successfully used to understand the concept of electron-pair localization in molecules and solids. The topological analysis of the ELF function enables the partitioning of the molecular space into ELF basins (core and valence basins, monosynaptic and polysynaptic) <sup>2</sup>. This is mainly based on the analysis of the gradient field of ELF, which is time-consuming and complex from an algorithmic perspective. Hence, there is a need for a rapid and easy identification of the nature of ELF basins. Our approach relies on the Independent Gradient Model (IGM) and its local descriptor  $\delta g$ .  $\delta g$  is a property of the Electron Density function that characterizes electron sharing between atoms when two or more electronic sources overlap. While zero values of  $\delta g$  correspond to monosynaptic basins, non-zero values correspond to polysynaptic basins. We implemented our approach within IGMPlot <sup>3</sup>, open-source freeware that is used to identify and quantify a broad range of molecular interactions. The ELF basins are analyzed using the  $qg$  descriptor, a descriptor that we had designed to enhance the IGM- $\delta g$  analysis. To illustrate and test our new analysis method, we selected about 100 typical systems. We calculated the ELF for each of these systems using IGMPlot. We compared our results with traditional ELF analysis methods using Topchem <sup>4</sup>. Our approach proved to be effective. It is worth mentioning that this new and very fast ELF<sup>&</sup>IGM analysis can be achieved with little preparation. It is therefore more suitable for pedagogical and practical use.

Figure 1. A 3D representation of the ELF isosurface of Ferrocene with IGMPlot



**Keywords:** Chemical bonds, Electron Localization Function (ELF), Quantum Chemical Topology (QCT), Electron Density (ED), IGMPlot.

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<sup>2</sup> B. Silvi and A. Savin, *Nature* 371 (1994) 683–686.

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<sup>4</sup> D. Kozłowski and J. Pilmé, *J. Comput. Chem.* 32 (2011) 3207–3217.