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**The Electron Localization Function (ELF): Applications to Some Main
Group and Transition Metal Molecules**

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Since its introduction in 1990 by Becke and Edgecombe, the electron localization function (ELF) has been acknowledged as a very useful tool for the analysis of wave functions. In 1994, Silvi and Savin generalized the atoms-in-molecules (AIM) topological approach pioneered by Richard Bader to ELF. The topological analysis of ELF has been applied to a large number of systems for which it provides a "chemical" picture of bonding. The ELF function is a local indicator of the Pauli repulsion strength and, therefore, its gradient field enables the molecular space to be partitioned into basins of attractors that correspond to VSEPR electron pair domains. A number of examples will be discussed including some hypervalent molecules such as SF₄, SF₄O and FPO₂ and transition metal halides such as TiF₃, MnF₃ and VF₃.

Dr. Stéphane Noury obtained a Licence (1992), Maîtrise (1993), Diplôme d'Etudes Approfondies (1994) and Doctorat (1999) from Université Pierre et Marie Curie, Paris, France. He has been a Postdoctoral Fellow with Prof. Ron Gillespie in the Department of Chemistry at McMaster University since July 1999. Using a combined atoms-in-molecules (AIM) and electron-localization-function (ELF) approach, the purpose of their work is to gain an understanding of why the geometries of transition metal halides do not agree with the VSEPR model. As ELF provides information on bonds and lone pairs, Dr. Noury is also using new topological approaches based on ELF to rationalize usual chemical concepts.

