Department of Chemistry

Departmental Seminar:

Physical, Computational & Materials Month

You are cordially invited to a virtual lecture presented by

Dr. Jurgens de Lange

Department of Chemistry, University of Pretoria

Date: Friday, 29th October 2021
Time: 10:30 – 11:20
Venue: Google Meet
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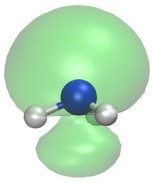
A couple of lonely electrons in a crowded room:

Revisiting the concept of an electron lone-pair

Modern conceptual chemistry often views electrons as highly correlated, *coupled* pairs of electrons: whether as bonding, dative or covalent pairs, antibonding isolated pairs or nonbonding localized lone-pairs, the concept of an electron pair is a ubiquitous foundation of chemistry. In addition to its importance *fundamentally*, the concept of electron pairs has tremendous *utility* in explaining chemical phenomena.

In particular, an electron lone-pair (LP) is an electron-pair localized to a single atom. LPs are, however, notoriously difficult to pin-down: an LP can easily be delocalized due to conjugation, hyperconjugation, induction, dative-covalency and dispersion. The effects of delocalizing an LP are also wide, ranging from geometrical changes (e.g. planar amine groups) to electronic (e.g. high-spin transition metal complexes). Clearly, the relative delocalization of LPs is a tuneable parameter in the rational design of materials and reactions.

Unfortunately, very few approaches exist which can quantify LP (de)localization, either theoretically or experimentally. We present an overview of the Fragment, Atomic, Localized, Delocalized and Interatomic (FALDI) density decomposition scheme. We show that FALDI can easily identify, quantify and visualize LPs, as well as trace their delocalization throughout a molecular system.



$\lambda^2_{\mathrm{LDO}}(\mathrm{N}) = 1.24\ \mathrm{e}^-$
Lone-pair electrons