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Electron Localization-Delocalization Matrices (LDMs): A Powerful Molecular Descriptor for in silico Design of Materials

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ABSTRACT

An electron localization-delocalization matrix (LDM) is a matrix representation of the complete molecular graph. A complete (molecular) graph links every pair of atoms (vertices) in the molecule - in contrast with the generally-incomplete chemical structure graph which only places a line between atoms considered to be chemically-bonded. The edges (links) of the graph represented by an LDM are electron delocalization channels which exist between every pair of atoms in the molecule (only a subset of these channels coincide with chemical bonds). An LDM, hence, contains information on the electron distribution in the molecule at an atomic/atomic-pair resolution. By feeding the matrix elements of the LDM with electron localization and delocalization indices calculated from numerical Quantum Theory of Atoms in Molecules (QTAIM), the LDM bridges quantum chemistry and chemical graph theory. Due to their sound foundations in physics, LDMs are powerful predictors of molecular and materials properties as diverse as pKa's, boiling points, substituents effects, aromaticity, corrosion inhibitors' activity (including discovery of the active species – Fig. 1), mosquito repellancy, UV λmax bathochromic shifts, enzyme catalysis, etc. [1-6]

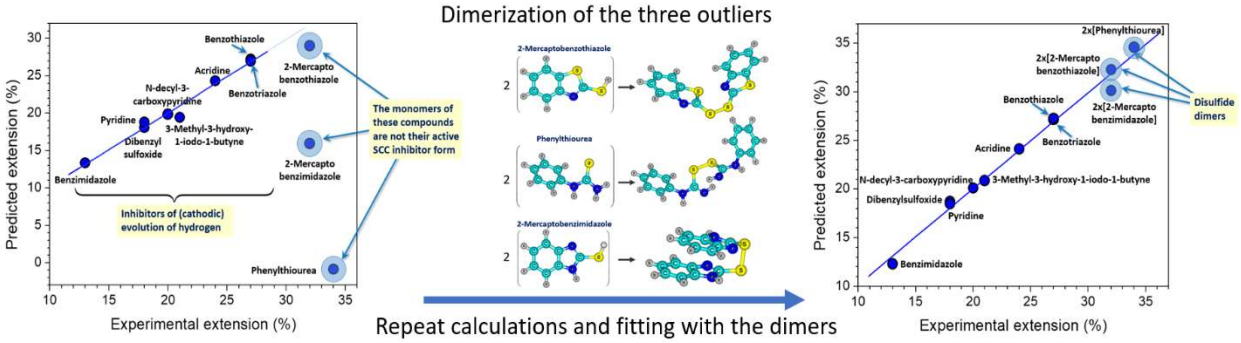

Fig. 1 LDM's PCA eigenvalues regressed against the experimental wire extension before breaking under stress corrosion cracking conditions showing how the inclusion of the correct species "normalizes" the three outliers with -SH groups after their oxidative dimerization at the anode. (Courtesy of Dr. Ronald Cook [1]).

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