# In Search of an Intrinsic Chemical Bond

*Amanda Morgenstern[1], Tim Wilson[1], Jonathan Miorelli[1], Travis Jones[1], Mark Eberhart[1]*

1. Molecular Theory Group, Colorado School of Mines

The chemical bond has meanings that change with context. In some contexts a bond is a physical connection between atoms, in others it is a energy lowering "bonding interaction". Which of these two connotations should be attached to the chemical bond has fostered considerable debate [1-5]. For example, the Quantum Theory of Atoms in Molecules (QTAIM) describes bonds as 1D ridges of charge density running between bound nuclei. While this definition provides an unambiguous definition of a bond as a physical link, it has been argued that these connections are not always energy lowering and hence do not correspond to bonding interactions. We have extended QTAIM by describing bonds more fully as 3D objects, called bond bundles, which are bounded by zero-flux surfaces in the gradient of the charge density [6]. This definition retains the topological elegance of a bond as an observable link between atoms, while, in turn, allowing one to associate with the bond bundle well defined properties, such as an energy. Furthermore, it is possible to decompose bond bundles into infinitesimal volumes, also bounded by zero-flux surfaces, and hence recover a property distribution of a bond bundle [7]. In our work to date, bond bundles have been used to analyze bonding interactions in small molecules [8], solid-state materials [9], and most recently, enzymes. The geometry of bond bundles has been found to correlate to reactivity. Finally, we are able to recover VSEPR diagrams of small molecules from the bond bundle electron density and kinetic energy distributions in smaller gradient bundles.
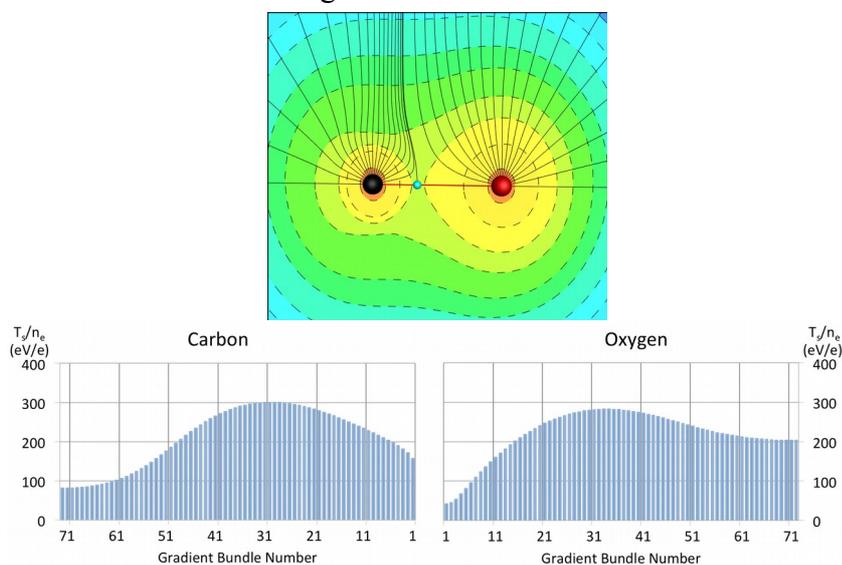


Top: Gradient paths seeded every 10º around C and O atoms in carbon monoxide. C-black, O-red. Bottom: Average kinetic energy per electron in each 2.5º gradient bundle for CO showing the distinct property distributions around each atom.

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