

Pushing molecules around: a theoretical perspective on the chemical bond, and how to modify it.

John McGrady

Department of Chemistry, University of Oxford

As students, we learn that chemical bonds can be either ionic, covalent, or perhaps somewhere in between. We also learn that bonds can be single, double, triple, and even quadruple, and the σ , π and δ components have their own characteristic structural preferences and reactivity patterns. These rather binary ideas about the chemical bond obscure the simple fact that all of chemical bonding involves the minimization of the total energy, which is in turn made up of kinetic and potential energies. The potential energy can be further subdivided into the attraction between electrons and nuclei, the repulsion between nuclei and the repulsion between electrons, and it is the latter that represents the major challenge to contemporary theories of bonding. When viewed in terms of the component parts, it is clear that bonding is in fact a continuum with no clear-cut divisions between different types, and our natural inclination as chemists to categorize and classify therefore offers a misleading perspective. In this talk I will show how the nature of the bonding in a range of different molecules, taken from both the transition series and the main group, can be changed quite dramatically by relatively minor perturbations including pressure, temperature, ionization and chemical substitution. The examples are drawn from collaborations with different experimental groups, and serve to illustrate the richness of the chemical bond.

