

Chemical bonding and reactivity: A local thermodynamic viewpoint

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The possibility of gaining insight into chemical bonding and reactivity through various local temperatures and associated entropy densities is explored. Comparisons of these quantities with other local reactivity descriptors like the electron density, the Laplacian of the density, the Fukui function and the electron localization function are made. The water molecule has been chosen as a prototype for analyzing the above-mentioned quantities. The global entropies are also calculated for the atoms He to Ne. Most of the local quantities preserve the molecular symmetry and some are well suited for use as reactivity indices.