

Bonding descriptors: reality or curiosity?

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The bonding in molecules or solids is an attribute used to describe the situation that the examined aggregate holds together at given conditions. This stability is of course controlled by the energy, usually determined from equations derived for a model system to simplify matters. To rationalize the interplay between the constituting atoms we characterize the overall bonding situation by means of different bonding descriptors and classify the interactions as a separate units called bonds. However, by doing so we encounter the uncomfortable task to analyze objects that are not observables. If the bonding descriptors are based on position dependent functions we cross (trespass on) the realm of quantum chemical topology. How real are the “real space” descriptors and do we just exploit the usefulness of the underlying model?