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Local energy: a basis for local electronegativity and local hardness

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The traditional approach to establishing a local measure of chemical hardness, by defining a local hardness concept through the derivative of the chemical potential with respect to the electron density, has been found to have limited chemical applicability, and has proved to be an unfeasible approach in principle. Here, we propose a new approach via a unique local energy concept. This local energy is shown to emerge from the Hamilton-Jacobi kind of construction of Schrodinger's quantum mechanics. It then leads to the concepts of a local chemical potential, i.e. negative of local electronegativity, and a local hardness just as the chemical potential and hardness are obtained from the energy, namely via differentiations with respect to the number of electrons. The emerging local hardness adds corrections to a recently proposed local hardness expression that has been found to be a good local measure of hardness for a series of atomic and molecular systems. These corrections become relevant for molecules with a large number of electrons. It is pointed out further that the definition of local softness that yields it as the Fukui function times the softness is not well-established, explaining recent observations of failure of this local softness concept as a proper local reactivity index for hard systems.

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