

The Fukui potential is a measure of the chemical hardness

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The chemical hardness is, after the chemical potential, the most important concept in describing the chemical reactivity of atoms and molecules. Recently, we showed that the Fukui potential at the nucleus of an atom is proportional to its hardness. Based on this, we speculated that the Fukui potential at the nucleus could be an alternative definition of the hardness. In this Letter we verify that the Fukui potential successfully describe the hardness of atoms. It is surprising that a property that depends only on the density at the nucleus can give such a good description of the chemical hardness. © 2011 Elsevier B.V. All rights reserved.