Links among the Fukui potential, the alchemical hardness and the local hardness of an atom in a molecule

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Abstract
This paper presents a brief summary of the difficulty that resides in the definition of the elusive concept of local chemical hardness. We argue that a definition of local hardness should be useful to a reactivity principle and not just as a mere definition. We then continue with a formal discussion about the benefits and difficulties of using the Fukui potential, which is interpreted as an alchemical derivative (alchemical hardness), as descriptor of local hardness of molecules. Computational evidence shows that the alchemical hardness is at least as good a descriptor as the combination of other two well-stabilized descriptors of local hardness, such as the Fukui function and grand canonical local hardness. Although our results are auspicious for the alchemical hardness as descriptor of local hardness, we finish by calling the attention of the community on the importance of discussing the raison d'être of a local hardness function and its main characteristics. We suggest that an axiomatic construction of local hardness could be they way of constructing a local hardness which is both useful and free of arbitrariness. © 2021 Wiley Periodicals LLC.

Author keywords
chemical reactivity; DFT; Fukui potential; local chemical hardness