An information-theoretic resolution of the ambiguity in the local hardness

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The ambiguity of the local hardness is resolved by using information theory to select definitions of the local hardness that are as close as possible to a well-defined approximate formula for the local hardness. A condensed local hardness is derived by using the atomic hardnesses as a reference distribution; a pointwise local hardness is derived by using the uniform electron gas as a reference distribution. This information-theoretic condensed local hardness is tested by examining electrophilic attack on some substituted pyridines. This journal is © 2014 the Owner Societies.