maximum hardness, principle of

A chemical system at a given temperature will evolve to a configuration of maximum absolute hardness, $\eta$, provided that the potential due to the nuclei, plus any external potential and the electronic chemical potential, remain constant. In terms of molecular orbital theory, the highest value of $\eta$ reflects the highest possible energy gap between the lowest unoccupied and highest occupied molecular orbitals; this value correlates with the stability (See: structural stability; electronic stability) of a system.

Source:
PAC, 1999, 71, 1919 (Glossary of terms used in theoretical organic chemistry) on page 1950