

# Reactivity indices and response functions in density functional theory

Fuentealba,

The hardness and softness quantities defined in density functional theory are discussed. A new scheme to calculate the hardness and softness hierarchies without resorting to the finite difference approximation is outlined. It is based in the relationship between the hardness and softness kernels and the linear response functions. As an example, the reactivity indices are extracted from an approximated model for the linear response function. © 1998 Published by Elsevier Science B.V. All rights reserved.