

# Introduction of external field effects in the frontier molecular orbital theory of chemical reactivity

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External field effects are introduced in both charge and orbital control terms of Klopman-Salem formalism for the study of chemical reactivity in condensed phase. An analytical expression is derived for the change of the interaction energy between a nucleophile and an electrophile from gas to solution phase. The resulting simple expression contains the effect of the external field, in terms of the variation of the electrophilic superdelocalizability index associated with the highest occupied molecular orbital (HOMO) of the nucleophile. Two classical reactions are analyzed to illustrate the usefulness and reliability of the proposed formalism. © 1992 John Wiley & Sons, Inc. Copyright © 1992 John Wiley & Sons, Inc.