# ADSORPTION OF ENANTIOMERS ON METAL SURFACES: APPLICATION TO D- AND L-ALANINE ON CU, NI AND ZN ELECTRODES

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## ABSTRACT

Different techniques have been developed for enantiomeric separation in order to meet the need for optically pure materials in the pharmaceutical, fine chemical and electronic industries. The present study explores the extent of selective adsorption of chiral compounds on metal electrodes, from knowledge of adsorption energy difference between D- and L- enantiomers. An entirely new simulation strategy is employed via Monte-Carlo method to evaluate the adsorption energy difference between D- and L- enantiomers. This methodology also yields the amount of each species adsorbed for a chosen electrode potential. The adsorption of tetrameric D- and L-alanines at Cu, Ni and Zn electrodes as well as in solution are studied using their stabilization energies obtained at the B3LYP/6-31G optimized structures. Subsequently these stabilization energies are employed as input parameters to estimate the adsorption energy difference between D- and L-alanine tetramers. The adsorption energy difference obtained from the simulation is found to be identical with the umbrella inversion energy for the lone pair of electrons on the amino group. It is demonstrated that, in a racemic mixture, only the D–alanine tetramer gets adsorbed predominantly on Cu, Ni and Zn while the adsorption of the L–species is more facile than the D-form when the corresponding pure enantiomer is employed. The origin of the preferential adsorption of D-enantiomer from a racemic mixture is interpreted using the computation of the molar volumes of the optimized geometries. Thus the evaluation of the adsorption energy of chiral compounds on metal electrodes can lead to valuable predictions for separation of optically active pure enantiomers.