Theoretical study of adsorbed molecules over ZnO surfaces.

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The interaction of small molecules with oxides is a continuous and growth area of interest. The performance of these studies is important for the innovation on materials science. ZnO presents a wide use, e.g., catalysis, chemical sensors, opto-electronics, and photoluminescence. Our main interest is the catalytic synthesis of methanol, and the hydrogenation of hydrocarbons. This study has the main objective of characterize the interaction of small molecules, e.g., CO, CO_2, H_2, and H_2O on ZnO surfaces. Zinc oxide has two mainly studied surfaces, the polar (0001) and (000-1) surfaces and the non polar (10-10) surfaces. These surfaces have specificity for some interactions. We have used the ONIOM hybrid method, using three layers: CCSD, PBE1PBE and UFF. The basis sets used for the ab initio methods are the 3-21G and the 6-31G* Pople basis. We have studied the interaction energies, BSSE corrections, population charges, orbital energies, and vibrational frequencies for the optimized structures.