Calculations for different adsorption states of acetylene on nickel

P. Geurts and A. van der Avoird
Institute of Theoretical Chemistry
University of Nijmegen
Nijmegen, The Netherlands

On the basis of different experimental information, UPS spectra, LEED data and EELS spectra, different bonding models for acetylene adsorbed on transition-metal surfaces, Ni, Pt, W (111), have been proposed (e.g. di-σ bonding, π-bonding, μ_3-bonding). By performing a series of Hartree-Fock-Slater LCAO calculations on C_2H_2 bonded to 1, 2 or 3 Ni atoms and correlation of the results with the experimentally observed adsorption shifts in the ionization energies and in the vibrational frequencies we attempt to characterize the different adsorbed states of C_2H_2.