DFT TEST STUDY ON VAN DER WAALS DIMERS

A. J. HERNANDEZ, M. C. SALAZAR, *Department of Chemistry, Simon Bolivar University, Caracas 1080A, Venezuela*; C. E. MANZANARES, *Department of Chemistry and Biochemistry, Baylor University, Waco, TX 76798*.

Studies in the framework of the supermolecule approach, using density functional theory with basis sets optimized for generalized gradient approximation exchange-correlation calculations, and constructed to give accurate values for nonbonding interactions, will be discussed. Bonding properties of the diatomic van der Waals $CO - He$ and $N_2 - He$ molecules will be presented and compared with recent experimental and theoretical results.