APOST-3D: A Program for Wavefunction Analysis

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APOST-3D units the programs AFUZZY and ENPART alongside with new features that have been added to the program in the last years. The main characteristic of APOST-3D is that it performs fast numerical integrations of one- and two-electron functions that can be easily split into atomic or diatomic domains. Nowadays it can perform integration over atomic domains using different atomic definitions such as, Mulliken, Löwdin, Hirshfeld, Hirshfeld-Iterative, Becke, Becke-rho, and QTAIM. The program can be used to compute charges, bond orders or delocalization indices, free-valences, energy partitions, local spins, effective atomic orbitals and oxidation states, conceptual DFT indices among other chemical properties. Moreover, APOST-3D generates atomic overlap matrices of the molecular orbitals that can be used by external programs to compute other properties such as aromaticity indexes (*i.e.,* ESI-3D by Eduard Matito). In this seminar I will make an overall presentation of the program highlighting the work that I have carried out over the last four years. The capabilities of the program will be illustrated with some examples.