ELECTRONIC STRUCTURE CALCULATIONS USING NONLINEAR BASIS EXPANSIONS

RON SHEPARD[a] and GERGELY GIDOFALVI, *Chemical Sciences and Engineering Division, Argonne National Laboratory, Argonne, IL 60439*.

Recent progress and applications using electronic wave functions expanded in a basis of nonlinear functions will be presented[b].

[b]R. Shepard, M. Minkoff, and S. R. Brozell, Int. J. Quantum Chem. 107, 3203 (2007)