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Abbreviation

DFT - Density functional theory

DNP - Double numerical plus polarization basis set

GGA - Generalized gradient approximation

VPSR - Perform all-electron calculation using scalar relativity

BSSE - Basis set superposition error

DIIS - Double inversion iterative subspace

BLYP - Becke Lee-Yang-Parr

SCF - Self consistent field (Self-consistent field, one of the principal calculation approaches comprising Hartree-Fock method in quantum chemistry)

NO – Nitrogen oxide

Pd - Palladium