Development of the all-electron mixed basis program, TOMBO

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We have developed the all-electron mixed basis approach (the name of our code is 'TOMBO') in which one-electron wave functions are expanded in a linear combination of both plane waves (PWs) and numerical atomic orbitals (AOs) confined inside non-overlapping atomic spheres (Fig.1a). The AOs are described as a product of the radial numerical function in logarithmic mesh and the cubic harmonics. A valence radial function is truncated by subtracting a smooth polynomial function that satisfies the matching condition at the surface of atomic sphere, while the rest smooth function (polynomial function inside and tail function outside atomic sphere) can be expressed by PWs (Fig.1b).

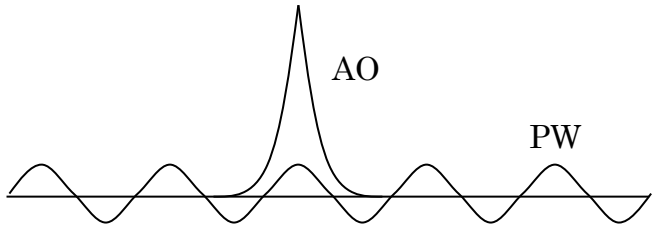

Fig.1a All-electron mixed basis representation of wave functions in a linear combination of AOs and PWs.

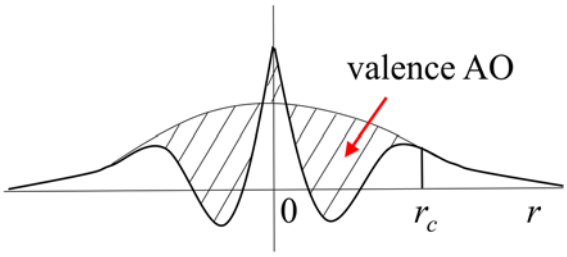

Fig.1b Valence AO is confined inside non-overlapping atomic sphere by subtracting a smooth polynomial function.

The method is free from the basis set superposition error (BSSE) and reduces the overcompleteness problem. Since neighboring AOs do not overlap, the related numerical error does not appear. The overlap between PW and AO are calculated by one-dimensional numerical integrations of a product of the spherical Bessel function and the radial numerical function. These treatments guarantee the accuracy of the computation. The method can well describe both deeply localized core orbitals and widely extended free-electron-like orbitals with relatively small number of basis functions, and is applicable to variety of systems including atoms, molecules, clusters, surfaces, interfaces, and crystals. TOMBO is now applicable to the calculations of (1)

molecular dynamics (MD) in density functional theory (DFT) (Fig.2) [1] or time-dependent (TD) DFT [2], (2) the dielectric or diamagnetic susceptibility of semiconductors or insulators (NMR chemical shift is under implementation) [3], (3) quasiparticle (i.e., photoemission) spectra in a framework of many-body perturbation theory, e.g., the *GW* approximation (Fig.3) [4], and (4) photoabsorption spectra [5] (or Auger spectra for the two electron emission process [6]) obtained by solving the Bethe-Salpeter equation (BSE) by beginning with the *GW* approximation. The program is fully parallelized by using openMP and MPI. We are now accelerating, debugging, and unifying the LDA part of TOMBO toward opening to the public in this fiscal year. Simultaneously, we are now distributing the executable module of the Windows β version of TOMBO. In this talk, we will explain the basic algorithms used in our code together with some recent results.

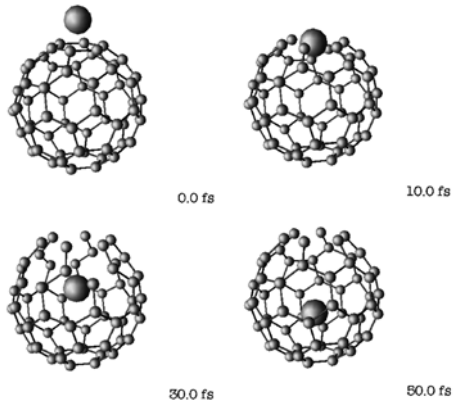

Fig.2 First-principles MD of Xe insertion into C_{60} [1].

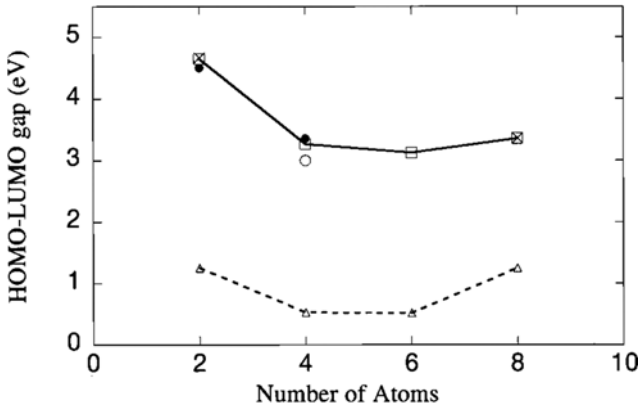

Fig.3 *GW* HOMO-LUMO gap of Na_n cluster [4].

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