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一般化並列 Elongation 法の開発と DNA・タンパク質への応用

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Introduction

At the *ab initio* level, the Generalized-Elongation (G-Elg) method has been applied to determining the electronic structures of linear water $(H_2O)_{12}$, two-dimensional $(H_2O)_{100}$ and the three-dimensional water cluster $(H_2O)_{20}$. When an attacking monomer is closed to any frozen regions, the G-Elg method can consider the strong interaction between these frozen regions and the attacking monomer by re-activating the frozen regions into the interactive region. Therefore, compared with the conventional calculations, the accuracy in total energy by the G-Elg can be reached in the order of 10^{-7} Hartree for any-dimensional systems.

Results and Discussion

One-dimensional water clusters $(H_2O)_{12}$ have been calculated by using the G-Elg, Old-Elg and conventional methods, as shown in Fig. 1. The procedures of the elongation method are described as the left side in Fig. 1. It can be seen from Fig. 1, because the strong interaction between the eleventh H_2O and the second H_2O, the energy difference calculated by the Old-Elg is abruptly increased when the eleventh water was involved. While for the G-Elg method, the energy difference is negligibly small because the second frozen water has been re-activated and included in the interactive space.

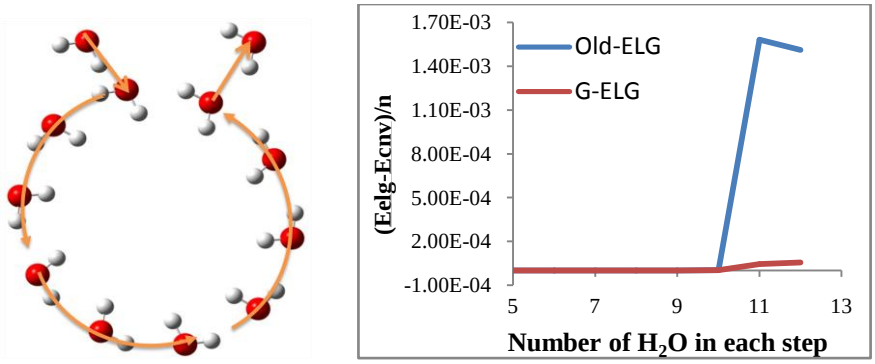


Fig. 1 The total energy difference between Old-Elg (blue line) and G-Elg (red line) for one-dimensional $(H_2O)_{12}$ calculated at HF/STO-3G level.

The two-dimensional water clusters have also been calculated by using the G-Elg method in this work, the total energy difference between the conventional and G-Elg calculations is shown in Fig. 2. In order to consider the strong interaction between the frozen region and the attacking monomer, any frozen units in 6 au, 10au, 15au and 20au around the attacking monomer will be re-activated, as shown in Fig. 2. As for different distances, the number of re-activated H_2O is given in Table 1. One can see from Fig. 2, with the increase of distance, the energy difference between the conventional and G-Elg calculations are decreased. Therefore, the G-Elg calculation can give the satisfactory results for two-dimensional system.

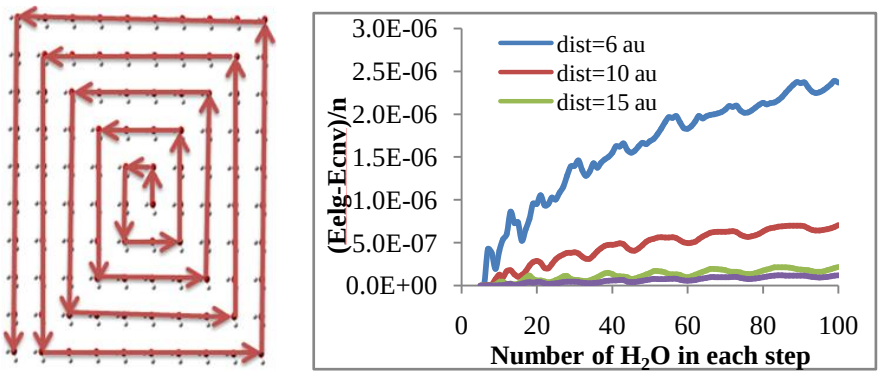
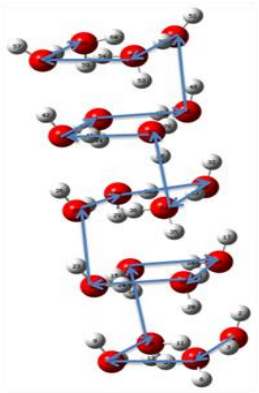


Fig. 2 The total energy difference between Old-Elg and G-Elg for two-dimensional $(H_2O)_{100}$ calculated at HF/STO-3G theoretical level.

Table 1. The number of re-activated H_2O in the elongation procedures

Distance (a.u.)	Number of re-activated H_2O
6	2
10	5
15	12
20	18

For the three-dimensional system, The stability energy (SE) of water cluster $(H2O)_{20}$ have also been calculated by using the G-Elg approach. The optimized geometry was taken from the work of Sathyamurthy et al[1] (as shown in Fig 3). Compared to the result of Sathyamurthy's, the stability energy calculated by the G-Elg method at HF/6-31G(d,p) level is in very good agreement.



SE(kcal/mol)	
Conv [1]	G-Elg
-216.28	-215.002

Fig. 3 The stability energy (SE) calculated by conventional and G-Elg methods for three-dimensional water cluster $(H_2O)_{20}$ at HF/6-31G(d,p) level

In the present work, we showed the effectiveness and efficiency of the G-Elg method for the one-dimensional, two-dimensional, and three-dimensional water cluster models. The application of the G-Elg method to other large biological systems of interests, such as protein or DNA is in progress in our lab.

Reference

[1] Maheshwary, S.; Patel, N. and Sathyamurthy, N., *J. Phys. Chem.* A 2001, **105**, 10525-10537.