Genetic Algorithm Approach for Nanoscale Devices

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Background: combinatorial problem

- Difficulty of Material Search by Combinatorial Approach
- To predict which molecules would be suitable
- It is currently very difficult to predict which molecules would be suitable for fabricating such devices, because the number of organic molecules that are available is enormous.
- One established approach is to use the computational methods developed for the prediction of a stable molecular structure and electronic properties.
- However, it is impossible to use a straightforward technique to evaluate these properties, because we have to do the calculations for a large number of candidate molecules.

For example, if a candidate organic molecule has **5 independent substitutional sites**, and if there are **10 (or 100) candidates** for substituents to interact with those sites, the possible number of combinations is **100,000 (or 10,000,000,000)**.

Why, GA (Genetic Algorithm)?

- To overcome this combinatorial problem, Genetic Algorithms (GA) were proposed by Holland in the 1970s [L. Davis, Handbook of Genetic Algorithms, (von Nostrand, New York, 1991).]. The main strategy of GAs is to imitate an evolution in nature by implementing “crossover” and “mutation” in a computer code.
- We propose that a Genetic Algorithm (GA) could be used to survey molecules to determine those which would be appropriate for practical molecular devices.
- In fact, this technique has already been adapted to optimize chemical structures and to evolve them to more useful compounds in the field of rational drug design [R. C. Glen and A. W. R. Payne, J. Comput. Aid. Mol. Des., **9** (1995) 181.].

Genetic Algorithm(GA) for Surveying of Organic Molecules

What is Genetic Algorithm (GA)?

Find best design in engineering problem

Find best solution in complicated real world problem

Analogy from nature, its evolution mechanism

population, mutation, crossover

The best individual will survive after long generation.

GA: A kind of optimization method.

To find x : F(x) → minimum

x mimics a gene.

⇨ Obtain a suitable x to evaluate F(x)

⇨ We can obtain minimization

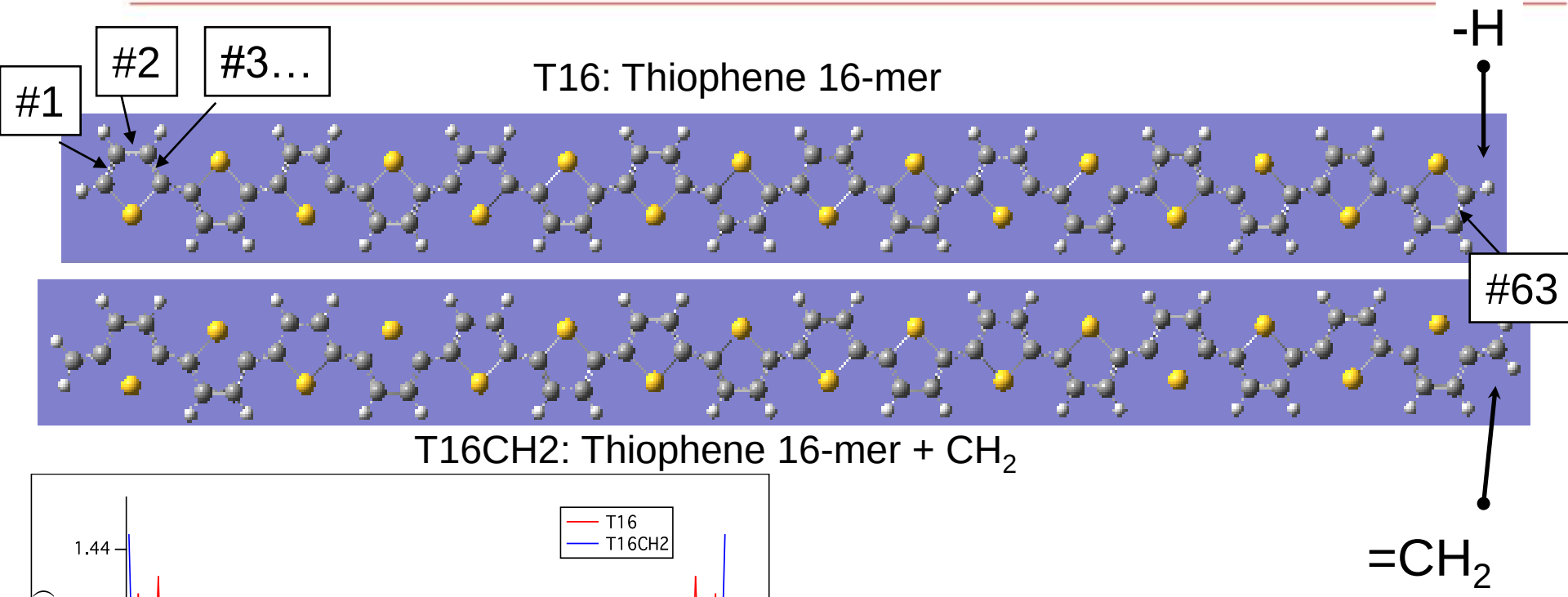
Advantage: We do not need to know F(x).

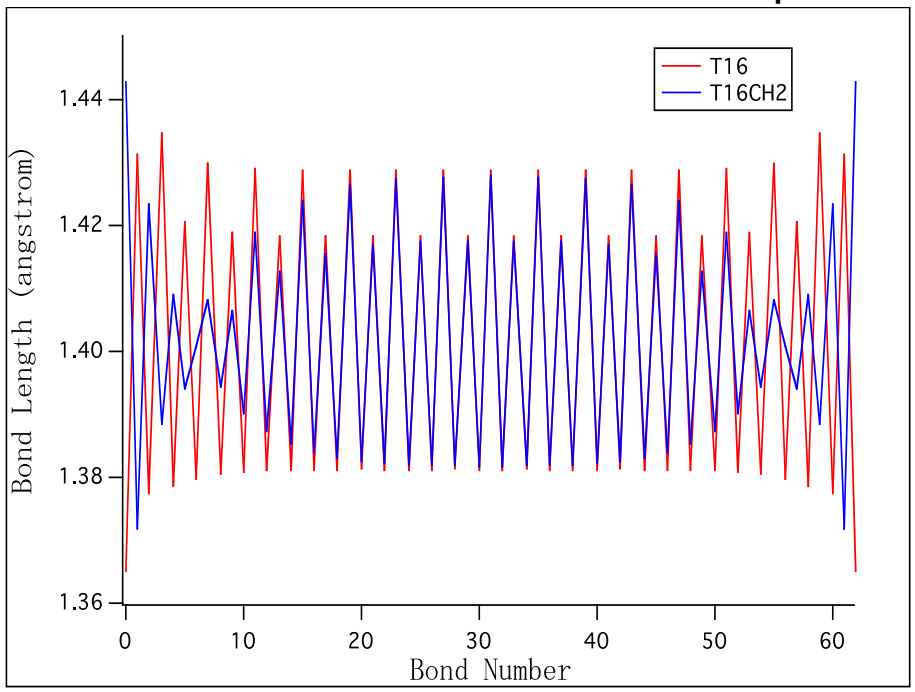
We can escape from a local minimum and survey the global minimum.

Disadvantage: We cannot say “This x is the global minimum”.

But, we can say “We hope this x is the global minimum”.

Oligo-Thiophene: -H or $=CH_2$





The energetics of the aromatic and quinoid structures is investigated using the both ends of neutral oligomers substituted by methylen is investigated.