

Project Title:

## Computationally assisted polymer synthesis

Name:

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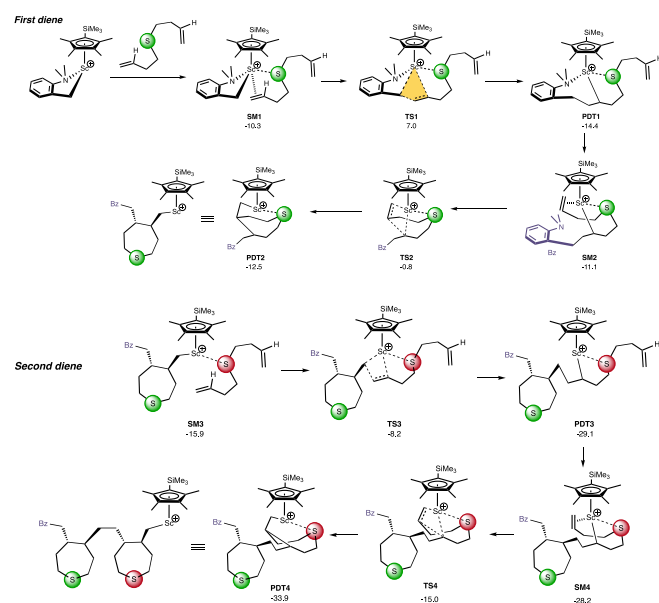
1. Background and purpose of the project, relationship of the project with other projects

The essence of chemical reaction is to study the interaction between electrons. How the microscopic electrons work needs to be simulated by supercomputers. With the aid of supercomputers, it plays a very important role in studying current chemical reactions, especially the simulation of polymers. Not only can understand the microscopic composition, but also can be used for the understanding of polymers and some dynamic properties, which is of great significance for the development and application of polymers

2. Specific usage status of the system and calculation method

Using Gaussian 16 to do the chemical structure optimization and transition state searching, to study the mechanism of the polymerization reaction.

3. Result



4. Conclusion

With the assistance of the HPC, we have been clearly understood the mechanism of this designing polymerization reaction. Next, we will carry out the experiment to realize this idea.

5. Schedule and prospect for the future

Next, we will conduct computational chemistry studies on more polymerization reactions.

6. If no job was executed, specify the reason.

None