H_2 Dissociation Discussions

Cheng Lab

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- 1 Introduction to Dissociation problem
- 2 Restricted Hartree Fock Solution
- 2.1 Discussion of results
- 3 Unrestricted Hartree Fock Solution
- 3.1 Discussion
- 4 Two Orbital two electron system
- 4.1 Spin Operator
- 4.2 Spin Adapted Configurations
- 5 Configurational Interaction Solution
- 5.1 Discussion
- 5.2 Secular Equations and its solution