

國立交通大學

應用數學系

碩士論文

原子虛位勢的 Ab Initio 計算

Ab Initio Computation for Atomic Pseudopotential



研究生：林浙于

指導教授：葉立明 教授

中華民國九十八年七月

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研究生：林浙于

Student : Che-Yu Lin

指導教授：葉立明

Advisor : Li-Ming Yeh

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碩士論文



A Thesis
Submitted to Department of Applied Mathematics
College of Science
National Chiao Tung University
in partial Fulfillment of the Requirements
for the Degree of
Master
in

Applied Mathematics

July 2009

Hsinchu, Taiwan, Republic of China

中華民國九十八年七月

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學生：林浙于

指導教授：葉立明

國立交通大學應用數學系（研究所）碩士班

摘要

我們用 ab initio self-consistent 方法計算出每一個原子的基態電子密度,然後再利用基態電子密度得出原子的基態總能.我們利用基態電子密度為基礎,構造出原子中每個電子組態的波函數所相對應的虛波函數,最後求得虛波函數的虛位勢.



Ab Initio Computation for Atomic Pseudopotential

student : Che-Yu Lin

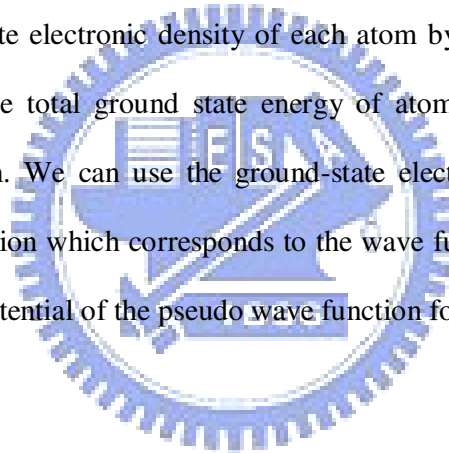
Advisors : Dr. Li-Ming Yeh

Department of Applied Mathematics

National Chiao Tung University

ABSTRACT

We calculate the ground-state electronic density of each atom by using ab initio self-consistent method, and then we obtain the total ground state energy of atoms from using the ground-state electronic density of each atom. We can use the ground-state electronic density of each atom to construct the pseudo wave function which corresponds to the wave function of valence states. In the end, we can obtain the pseudopotential of the pseudo wave function for each angular momentum.



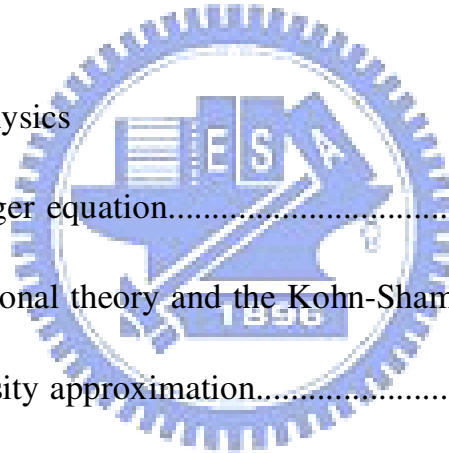
誌 謝

非常感謝我的指導教授,對於我研究上的問題,不厭其煩的為我解答,陪我一起成長,無以回報,並且謝謝各位口試委員的指導,還要感謝陪我一起奮鬥的同學,在遇到困難或灰心的時候,給我鼓勵和支持,我的家人也是對我不遺餘力的支持,如果沒有這些幫助我的人,我也不能順利的完成學業,對此,我感恩於心。



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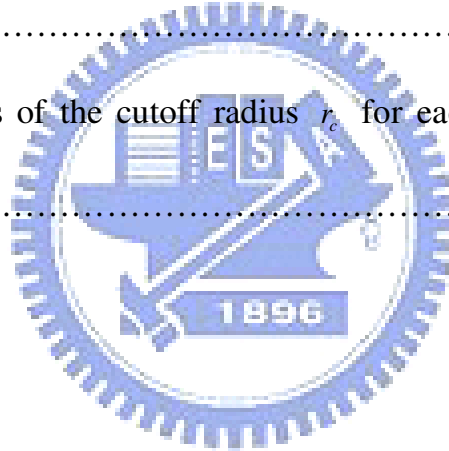


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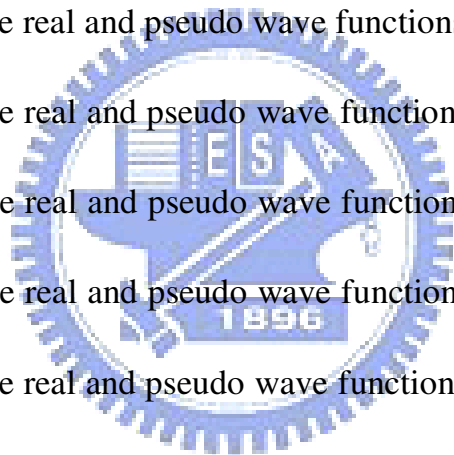


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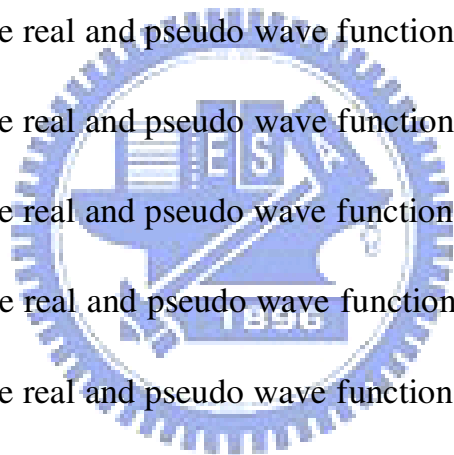


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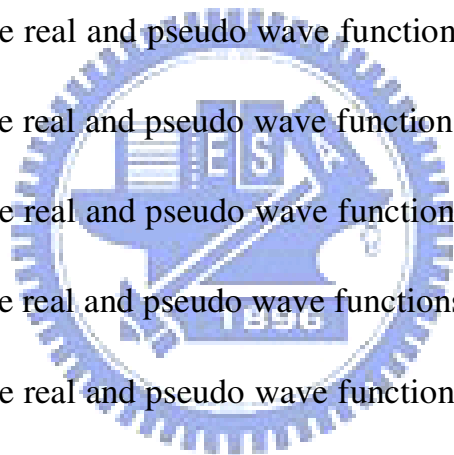


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