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QUANTUM MECHANICAL STUDY OF SOME LASER COLOR CENTERS AND ADSORPTIVITY AT METAL OXIDE SURFACES

A thesis

Submitted to the Faculty of Science
Zagazig University- Benha Branch
In Partial Fulfillment of the Requirement for the Degree of
Master in Science (Chemistry)

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2002

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**QUANTUM MECHANICAL STUDY OF SOME
LASER COLOR CENTERS AND ADSORPTIVITY
AT METAL OXIDE SURFACES**

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بِسْمِ اللَّهِ الرَّحْمَنِ الرَّحِيمِ

"وقل إعملوا فسيرى الله عملكم ورسوله والمؤمنون"

صدق الله العظيم

ACKNOWLEDGMENT

I am deeply thankful to Allah by the grace of whom the progress and success of this work was possible.

I am also, indebted with sincere gratitude to *Prof. Dr. Ahmed S. Shalabi*, Prof. of Theoretical Chemistry, Faculty of Science, Zagazig University, Benha Branch, for suggesting the research problem, critical continuous supervision and helpful guiding.

My indebtedness and sincere gratitude are also to *Dr. Tomador F.F. EL-Essawy* Assistant Prof. of Physical Chemistry and *Dr. Mervat M. Assem* Lecturer of Theoretical Chemistry Faculty of Science, Zagazig University, Benha Branch, for support, encouragement, and continual guidance.

Finally, I would like to express my everlasting gratitude and respect to my husband and my parents for their unlimited patience, continuous support and encouragement.

Abbreviations and Acronyms

Symbol	Acronyms
AO	Atomic Orbital.
BSSE	Basis set superposition Error.
CI	Configuration interaction.
CIS	Configuration interaction including single Excitations.
CISD	Configuration interaction including single and double Excitations.
CB	Conduction Band.
DF	Density Functional.
HF	Hartree –Fock.
HOAO	The Highest Occupied Atomic orbitals.
HOMO	The Highest Occupied Molecular orbitals.
LUAO	The Lowest Unoccupied Atomic orbitals.
LUMO	The Lowest Unoccupied Molecular orbitals.
MO	Molecular Orbitals.
RES	Relaxed Excited State.
SCF	Self- Consistent Field.
SEE	Size Extensivity Error.
STO	Slater Type Orbitals.
TD	Time Dependent Hartree-Fock and Density Functional Theory.
VB	Valence Band.

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