
شبكة المعلومات الجامعية


# بسم الله الرحمن الرحيم


# شبكة المعلومات الجامعية

# التوثيق الالكتروني والميكروفيلم

شبكة المعلومات الجامعية

# جامعة عين شمس

التوثيق الالكتروني والميكروفيلم

## قسم

نقسم بالله العظيم أن المادة التي تم توثيقها وتسجيلها
علي هذه الأفلام قد أعدت دون أية تغيرات

## يجب أن

تحفظ هذه الأفلام بعيدا عن الغبار

في درجة حرارة من ١٥-٢٥ مئوية ورطوبة نسبية من ٢٠-٤٠%

**To be Kept away from Dust in Dry Cool place of 15-25- c and relative humidity 20-40%**

# بعض الوثائـــــــق الاصليـــــة تالفـــة

# بالرسالة صفحات لم ترد بالاصل

Ain Shams University
Faculty of Education
Physics Department

Title of thesis



# *Theoretical study of Defects In Ionic crystals*

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# Contents

# AIM OF STUDY

The aim of the present study is twofold. First, to report the results of the first calculations of the doublet ground state configurations of the self trapped hole (STH) in LiH, the results of the UHF-SCF and MP2 calculations on an electronically inert (001) surface of an insulator LiH, and the effect of introducing the surface STH on modifying the nature of adsorbate-substrate interaction. Second, to examine how close are the energetic properties of the bulk and surface orientations of STH in LiF and NaH isoelectronic crystals, and how close are the energetics of atomic H adsorption and band structure of the relevant surfaces.

# Abbreviations and Acronyms

| Symbol | Acronyms |
|---|---|
| HOMO | Highest Occupied Molecular Orbital. |
| LUMO | Lowest Unoccupied Molecular Orbital. |
| SOMO | Singly Occupied Molecular Orbital. |
| SOAO | Singly Occupied Atomic Orbital. |
| STH | Self –Trapped Hole. |
| STE | Self-Trapped Exciton. |
| LDOS | Local Densities Of States. |
| $E_{ads}$ | Adsorption Energy. |
| $MP_2$ | Møller-Plesset Second orders perturbation correction. |
| UHF | Unrestricted Hartree Fock |
| ICECAP | Ionic Crystal with Electronic Cluster: Automated Program. |
| RHF | Restricted Hartree Fock |
| SCF | Self-consistent Field. |

# LIST OF FIGURES

# LIST OF TABLES

(3.2) Data for the adsorptivity of atomic H on the defect free and On-STH defect containing surfaces of LiF and NaH. 79

Δ: substrate site.,

$R_e$: equilibrium adatom substrate distance in Å.

$E_{ads.}$ : adsorption energy in eV.