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شبكة المعلومات الجامعية التوثيق الالكتروني والميكروفيلم



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Theoretical study of Defects In Ionic crystals

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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.

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Δ : substrate site.,

R_e : equilibrium adatom substrate distance in Å.

E_{ads} : adsorption energy in eV.

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