

12

AD-A184 276

OFFICE OF NAVAL RESEARCH

Contract N00014-86-K-0304

R&T Code 413F0005

Technical Report No. 3

DTIC
SELECTED
SEP 01 1987
S D
CLD

Valence Bond Cluster Studies of Alkali Metal/Semiconductor Bonding

by

R.C. Tatar and Richard P. Messmer

Abstract Submitted

for the March 1987 Meeting of the

American Physical Society

University of Pennsylvania
Department of Physics
Philadelphia, PA

December 1986

Reproduction in whole or in part is permitted for
any purpose of the United States Government

* This document has been approved for public release
and sale; its distribution is unlimited.

*This statement should also appear in Item 10 of the Document Control Data-DD
Form 1473. Copies of the form available from cognizant contract administrator.

1 508

Abstract Submitted
for the March 1987 Meeting of the
American Physical Society

December 1, 1986

23a

Valence Bond Cluster Studies of Alkali
Metal/Semiconductor Bonding R.C. Tatar, Univ. Penn.;
R.P. Messner, General Electric CRD and Univ. Penn. We
present results of cluster studies of alkali
metal/semiconductor bonding. Using the Generalized
Valence Bond (GVB) method, we find a remarkable con-
sistency in the behavior of bonding orbitals for a
variety of systems, including: LiH, Cl_4 , LiH_4 and
several "hypervalent" systems, such as SiH_3Li_2 , SiH_4Li_2 .
Our results show that the metal-semiconductor bonding in
these systems can be understood in terms of a pairing
between McAdon-Goddard type* metallic bonding orbitals
and a set of equivalent orbitals of the non-metallic
species. We propose that the results are relevant to
the initial stages of alkali overlayer growth on sem-
iconductor surfaces and lead to a simple picture of the
bonding including the transition from a non-conducting
to a conducting layer. We have considered numerous pro-
posed "hypervalent" structures in light of the above
results and find that they can be understood in terms of
more conventional concepts of valency. From these
results we conclude that the concept of "hypervalency"
needs to be refined, if not discarded. This work was
supported in part by the Office of Naval Research.

* M.A. McAdon, W.A. Goddard III, PRL 55, 2563 (1985).

Robert C. Tatar

Robert C. Tatar

Department of Physics
University of Pennsylvania
Philadelphia, PA 19104

Accession For	
NTIS CRA&I	<input checked="" type="checkbox"/>
DTIC TAB	<input type="checkbox"/>
Unannounced	<input type="checkbox"/>
Justification	
By _____	
Distribution/	
Availability Codes	
Dist	Avail and/or Special
A-1	

QUALITY
INSPECTED
2

Copy available to DTIC Agencies
without further request