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Theoretical analysis of semiconductor surface passivation by adsorption of alkaline-earth metals and chalcogens

By: Srivastava, GP (Srivastava, G. P.)^[1]; AlZahrani, AZ (AlZahrani, A. Z.)^[2]; Usanmaz, D (Usanmaz, D.)^[3]

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Abstract

We begin with the concept of semiconductor surface passivation by adsorption of sub-monolayer atomic coverages. We then present a theoretical analysis of structural reconstruction and passivating behaviour of semiconductor surfaces upon sub-monolayer adsorption of alkaline-earth metals (group II atoms) and chalcogens (group VI atoms). Specific results are presented from first-principles calculations for Ca adsorption on Si(0 0 1) and Si(1 1 1), and S adsorption on GaAs(0 0 1). The role of chemical species of adsorbate and surface atoms in achieving different degrees of passivation is highlighted. (c) 2012 Elsevier B.V. All rights reserved.

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Author Information

Reprint Address: Srivastava, GP (reprint author)

+ Univ Exeter, Sch Phys, Stocker Rd, Exeter EX4 4QL, Devon, England.

Addresses:

+ [1] Univ Exeter, Sch Phys, Exeter EX4 4QL, Devon, England

+ [2] King Abdulaziz Univ, Dept Phys, Jeddah 21413, Saudi Arabia

+ [3] Middle E Tech Univ, Phys Program, KKTC, TR-10 Guzelyurt, Mersin, Turkey

E-mail Addresses: gps@excc.ex.ac.uk

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