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

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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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