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SİLİCENE SENSÖRLER: TEORİK ARAŞTIRMA

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ABSTRACT

Silicene Sensors: Theoretical Investigations

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Two dimensional hexagonal structure of silicon, namely, silicene is nonmagnetic semimetal as reported previously. Silicene has massless Dirac Fermions due to linear dispersion around Fermi level at symmetric point K and $K^{'}$ in the reciprocal lattice. As a result, trembling motion of charge carriers, Klein Tunneling, high mobility of charge carriers, ambipolar effect, and anomalous quantum Hall effect can be observed in silicene. The silicene structure is not stable in planar geometry due to mixed sp^2 - sp^3 hybridization, so its stable form is a buckled honeycomb structure with 0.44 Å buckling [1]. Due to weaker π coupling compared to graphene, silicene is able to form strong bonds with metal atoms. Therefore, electronic and magnetic properties of silicene can be modified through adatom adsorption.

In this thesis, we investigate the atomic and electronic properties of bare, Ag_n (n=1-3) adsorbed silicene structure in view of first principles calculations. Also, we investigate the atomic and electronic properties of Pt substitution and adsorption on silicene. After that interaction of Pt adsorbed and substituted on Silicene with C, H, O atoms and CH_4, CO_2, O_2, H_2 molecules is examined in detail. Among the several studies, we haven ’t encountered any study investigating the silver (Ag) adsorption on silicene sheet in detail. Silver atoms and Platinum atom have high degree of antimicrobial activity, thermal stability as well as high catalytic property. So it is important to examine the electronic changes in silicene upon interaction with Ag and Pt. We believe that our results are crucial for understanding the fundamental process of interaction between silver and silicene at atomic scale.

Key Words
DFT (Density Functional Theory), Silicene, Sensors.