INTISARI

EFEK *STRAIN* TERHADAP SIFAT ELEKTRONIK *SILICENE* : KAJIAN KOMPUTASI BERBASIS DFT (*DENSITY FUNCTIONAL THEORY*)

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Telah dilakukan kajian komputasi berbasis *density functional theory* (DFT) pada material 2D silikon yaitu *silicene*. Setelah dibuktikan adanya perilaku *'massless Dirac fermion'* dan struktur geometri *buckle* pada keadaan optimal, pemberian *strain* dua-sumbu secara *compressive* atau *tensile* telah merubah struktur elektronik dan *buckle silicene*. Perubahan nilai *buckle* semakin besar atau kecil tergantung apakah dikenai *compressive* atau *tensile strain*. Perubahan struktur elektronik terjadi pada strain $\pm 8\%$ karena kenaikan energi *valence band* dan penurunan energi *conduction band* sehingga pada *strain* $\pm 8\%$ pita energi pada simetri$-\Gamma$ dan simetri$-K$ saling *overlap* yang mengakibatkan *silicene* menjadi konduktor, *overlap* energi semakin besar hingga *strain* -10% dan +12% yaitu 0,7650 eV dan 1,0326 eV. *Strain* -10% mengakibatkan konstanta *buckling* semakin besar menjadi 0,8467 Å sementara *strain* +12% mengakibatkan konstanta *buckling* semakin kecil menjadi 0,1994 Å.

Kata-kata kunci : *Silicene*, DFT, *Dirac fermion*, *strain*.

ABSTRACT

EFFECT APPLIED STRAIN AGAINTS ELECTRONIC PROPERTIES OF SILICENE : COMPUTATIONAL STUDY BASED ON DFT (DENSITY FUNCTIONAL THEORY)

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Computational study based on density functional theory (DFT) has been investigated for 2D silicon atoms : silicene. After massless Dirac fermion characteristic and buckle geometry structure on optimal parameter have been proved, applied biaxial strain as compressive and tensile has changed electronic properties and geometry structure silicene. The changed values of buckling will increase or decrease whether those are applied as the compressive or tensile strain. The changed electronic structure is applied strain $\pm 8\%$ because shifted valence band and conduction band into Fermi level, as the result energy band on Γ-point and K-point overlap and finally silicene as a conductor, overlap energy will increase until applied strain -10% and +12% about 0.7650 eV and 1.0326 eV respectively. Strain -10% yield buckling constant will increase to 0.8467 Å while strain +12% yield buckling constant will decrease to 0.1994 Å.

Keywords : Silicene, DFT, Dirac fermion, strain.