Uniaxial Strain on Graphene: Raman Spectroscopy Study and Band-Gap Opening [*ACS Nano* **2008,** *2,* 2301–2305]. Zhen Hua Ni, Ting Yu, Yun Hao Lu, Ying Ying Wang, Yuan Ping Feng, and Ze Xiang Shen*

In this article, we proposed that a gap can be opened by applying a uniaxial strain on graphene based on results of our density functional theory (DFT) calculations. However, we realized that this conclusion is incorrect and it was a result of overlooking the slight shift of the Dirac cone from the special *K* or *K*′ point in the reciprocal space. Figure 1 shows (black squares) the correct variation of energy gap at the Dirac point. Graphene remains gapless until the uniaxial strain along the zigzag direction (lower-left inset) reaches about 26.5%, which is in agreement with a recent tight-binding calculation (Pereira, V. M.; Castro Neto, A. H.; Peres, N. M. R. A Tight-Binding Approach to Uniaxial Strain in Graphene. Reprint in arXiv:0811.4396, **2008**). The two Dirac cones at *K* and *K*′ move toward each other as the strain increases (upper-right inset) and merge at the above critical strain (blue triangles). Beyond this critical strain, an energy gap opens at the Dirac point. However, the edge (at the *M* point of Brillouin zone) of another conduction band is lowered as the strain increases and drops below the valence band edge at the above critical strain (red circles), effectively closing the gap. Thus, based on results of DFT calculations, applying a uniaxial strain to graphene may not open a band gap.

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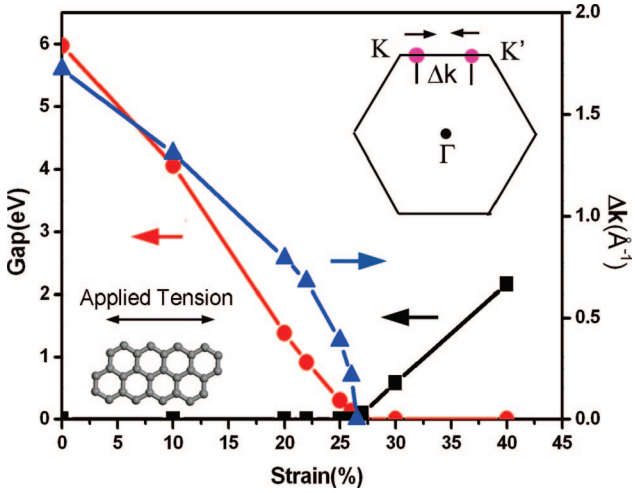

Figure 1. Energy gap at the Dirac point (black squares), minimum energy (at *M*) of the conduction band which shifts downward with strain (red circles), and separation between *K* and *K*′ (Δ*k*, upper-right inset, blue triangles) as a function of strain along the zigzag direction (lower-left inset). The Fermi level is set to zero.

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