Energetics and Electronic Structure of Scrolled 2D Materials

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Atomic layer materials can form various conformations, such as tubular, scrolled, and wrinkled conformations, because of their dimensionality and stable covalent networks. These structural conformations of atomic layer materials cause unique physical properties owing to the curvature and dimensionality. In particular, the curvature occasionally causes the unique electronic structure near and at the Fermi level [1,2]. Among the such conformations, scrolled atomic layer materials are very unique materials where the self-interaction via interlayer interaction plays crucial role to determine their electronic properties [3,4]. Thus, I this work, we aim to investigate the energetics and detail electronic structure of scrolled graphene sheet in terms of their diameter of inner most shell using the density functional theory with local density approximation.
Our calculations demonstrated that the scrolled graphene possesses unique electronic structures reflecting their curvature and interlayer self-interaction. The scrolled graphene consisting of zigzag graphene nanoribbon is a semiconductor with a tiny gap between its edge states around the Brillouin zone boundary, because of the electrostatic potential difference between inner and outer edges. Furthermore, the band edges of the scrolled graphene show the spatial dependence whether the shell is located at inner, middle, and outer portions in the scroll (Fig. 1).

References

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Figures

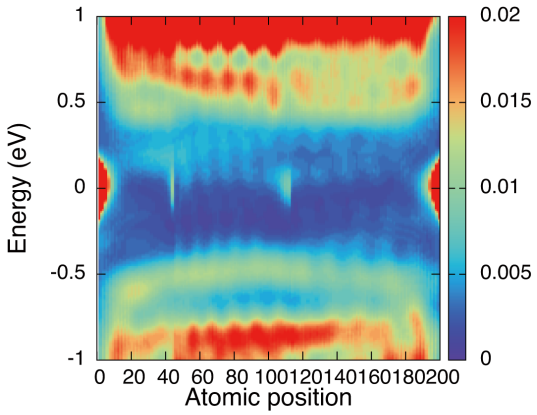

Figure 1: Projected density of states of C atoms at the innermost (position 1) to the outermost (position 200) on the graphene nanoscroll.