Geometric and electronic structures of diamond nanowires

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Diamond has been expected to be applicable to the high-power and high-frequency electronic devices, because of its excellent electronic and thermal properties, such as the wide band gap, high thermal conductivity, high breakdown field and high carrier mobility. Accordingly, diamond nanowires (DNWs) have also attracted much attention, because they have a potential to miniaturize the diamond-based devices. In addition, they are expected to exhibit novel properties which are absent in bulk diamond. Both top-down and bottom-up approaches was used to synthesize DNWs with diameters of 50-100 nanometer and of sub-nanometer, respectively. In this work, we aim to theoretically explore the geometric and electronic structures of DNWs with diameters of 0.5 nanometer, in terms of their shape and surface termination, based on the density functional theory combined with the effective screening medium method.

Here, we consider DNWs along (111) direction which have triangular and hexagonal cross sections with hydrogenated and clean side-walls, respectively. Our calculations showed that DNWs with the hydrogenated surfaces kept their initial shapes indicating that C atoms retain sp^3 hybridization, while DNWs with the clean surfaces exhibited significant surface reconstructions causing the modulation of their cross section due to the presence of dangling bonds on the surfaces. The electronic property of the DNWs also depends on their surface termination and the cross section. The DNWs with the hydrogenated surfaces are semiconductors with a direct energy gap of 3.92 and 3.67 eV at the Γ point for the nanowire with the triangular and hexagonal cross section, respectively. In contrast, the DNWs with the clean surfaces are metals irrespective of the cross section. In addition to the static electronic properties, we also studied the electronic properties of DNWs under an external electric field. We found that electrostatic potential inside the DNWs strongly depends on their surface terminations.

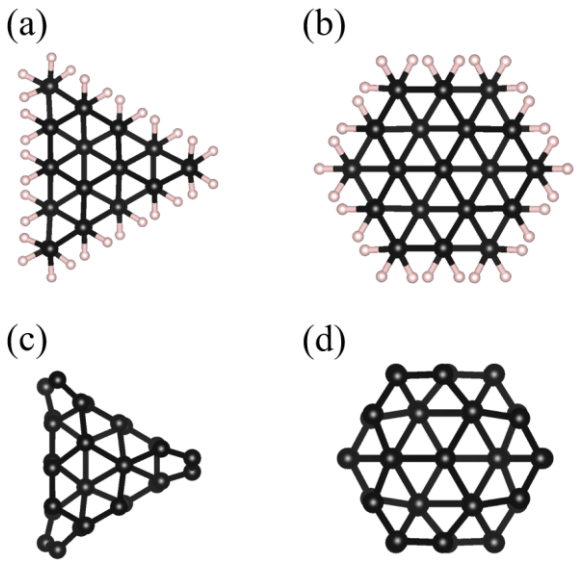

Fig. 1 Optimized geometric structures of hydrogenated-surface DNWs with the (a) triangular and (b) hexagonal cross section and clean-surface DNWs with the triangular and (d) hexagonal cross section.