Lei Tao (陶蕾)[1,2]

Yu-Yang Zhang (张余洋)[1,2,3], Jiatao Sun (孙家涛)[1,2], Shixuan Du (杜世萱)[1,2,3†] and Hong-Jun Gao (高鸿钧)[1,2,3]

[1]Institute of Physics, Chinese Academy of Sciences, Beijing 100190, China
[2]University of Chinese Academy of Sciences, Beijing 100190, China
[3]CAS Center for Excellence in Topological Quantum Computation, Chinese Academy of Sciences, Beijing 100190, China

ltao@iphy.ac.cn

Band engineering of double-wall Mo-based hybrid nanotubes

Hybrid transition-metal dichalcogenides (TMDs) with different chalcogens on each side (X-TM-Y) have attracted attentions because of the unique properties. Nanotubes based on hybrid TMD materials have advantages in flexibility over conventional TMD nanotubes. Here we predict the wide band gap tunability of hybrid TMD double-wall nanotubes (DWNTs) from metal to semiconductor. Using density-function theory (DFT) with HSE06 hybrid functional, we find that the electronic property of X-Mo-Y DWNTs (X = O and S, inside a tube. Y = S and Se, outside a tube) depends both on electronegativity difference and diameter difference. If there is no difference in electron negativity between inner atoms (X) of outer tube and outer atoms (Y) of inner tube, the band gap of DWNTs is the same as that of the inner one. If there is a significant electronegativity difference, the electronic property of DWNTs ranges from metallic to semiconducting, depending on diameter differences. Our results provide alternative ways for the band gap engineering of TMD nanotubes.

References

[1] Lei Tao, Yu-Yang Zhang, Jiatao Sun, Shixuan Du, Hong-Jun Gao, Band engineering of double-wall Mo-based hybrid nanotubes, Chinese Physics B, Vol. 27, No. 7, 2018.