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Quantum Simulation of SiC Nanotubes

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Abstract - We performed a series of quantum simulations for the geometrics, electronic structures and electron transport of various types of silicon carbide nanotubes (SiCNT's). The 1:1 SiCNT's generally show more stable semi-conducting behavior than carbon nanotubes (CNT's). The SiCNT's exhibit better electronic properties than their bulk materials. Their band gap increases with increasing the tube diameter. Armchair SiCNT's have narrower band gap than zigzag ones, whereas the zigzag SiCNT's possess direct band gap.

Keywords**:** Silicon carbide nanotubes, Quantum simulation, Electronic structures, Band gap, Electron transport