Mechanical strain can switch the sign of quantum capacitance from positive to negative

Li, Xiaobao, xli37@uh.edu; Sharma, Pradeep, University of Houston, United States

ABSTRACT

Quantum capacitance is a fundamental quantity that can directly reveal many interactions among electrons and is expected to play a critical role in nanoelectronics. One of many tantalizing recent physical revelations about quantum capacitance is that it can possess a negative value, hence allowing for the possibility of enhancing the overall capacitance in some particular material systems beyond the scaling predicted by classical electrostatics. Using detailed quantum mechanical simulations, we find an intriguing result that mechanical strains can tune both signs and values of quantum capacitance. We use a small coaxially-gated carbon nanotube as a paradigmatical capacitor system and show that, for the range of mechanical strain considered, quantum capacitance can be adjusted from very large positive to very large negative values (in the order of plus/minus hundreds of at-to farads), compared with the corresponding classical geometric value (0.31035 aF). We elucidate the mechanisms underpinning the switching of the sign of quantum capacitance due to strain. This finding opens novel avenues in designing quantum capacitance for applications in nanosensors, energy storage, and nanoelectronics.