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Electron Transport in Fluorinated Singe Wall Nanotubes<sup>1</sup> THUSHARI JAYASEKERA, JUNWEN LI, JOHN W. MINTMIRE, Oklahoma State University, VINCENT MEUNIER, Oak Ridge National Laboratory — Taking advantage of helical symmetry, we present results for the electronic structure and electron transport properties of fluorinated chiral single-wall carbon nanotubes, within an all-electron, local density functional approach. In this talk, we discuss the effect of pairs of fluorine substituents on metallic nanotubes. Our results show that this fluorination results in resonance features in the vicinity of the Fermi level. The resonance behavior comes out as a result of the interaction of the C-C atoms those are close to the F-attached C atoms. We also discuss the change of atomic structure caused by fluorination. To our knowledge this is the first electron transport calculation that uses the helical symmetry within a first-principles approach. We find that the use of helical symmetry has important advantages in electron transport calculations of systems with local defect sites. We will also briefly discuss about the application of this technique on Si nanowire systems with defects.

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