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Electronic properties of double-wall carbon nanotubes and the effect of functionalization[1] JONATHAN LAFLAMME JANSSEN, JASON BEAUDIN, MICHEL CÔTÉ, Département de Physique and Regroupement québécois sur les matériaux de pointe (RQMP), Université de Montréal, Canada, MICHEL COTE TEAM — Although promising for many electronic applications, further understanding of carbon nanotubes systems are required for practical designs. A difficulty currently hindering further development in this field is the considerable degradation of transport properties in a single-wall carbon nanotube (SWCNT) when it is subjected to ambient conditions or functionalized. Double-wall carbon nanotubes (DWCNT) could solve this problem, by allowing the outer tube to be functionalized while the inner tube would retain a pristine structure and it's promising electronic properties. However, our understanding of interactions between the tubes and their consequences on the system's electronic properties is still incomplete. In this presentation, we investigate those interactions using density-functional theory (DFT) calculations. In particular, we investigate separately the effects of structural deformations, Fermi energy realignment and electronic orbital overlap on the band structure of DWCNT. The effects of functionalization will also be addressed.

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