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Ab initio study of the dependence of the reactivity upon carbon nanotube diameter JONATHAN LAFLAMME JANSSEN, JASON BEAUDIN, MICHEL CÔTÉ, Département de physique, Université de Montréal, Canada, NICHOLAS D.M. HINE, PETER D. HAYNES, Imperial College, London, United Kingdom — One of the main research efforts of the recent years has been the development of an efficient way to select desired carbon nanotubes according to their size and their electronic properties. This selectivity would allow easier fabrication of field effect transistor and light-emitting diode devices with appropriate nanotubes. An appealing approach to assess this problem is to use the dependence of chemical functionalization thermodynamics on the material's properties. In this talk, ab initio studies of carbon nanotubes functionalized with bromophenyl will be presented. The radius dependence of the binding and activation energies of this functionalization will be reported. The purpose of this presentation is also to demonstrate the performance of linear-scaling density-functional theory code ONETEP, which provides the possibility carrying out large system simulations (up to several tens of thousands of atoms). Furthermore, the diameter dependence of the oxidation of carbon nanotubes by carbon dioxide will be presented.

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