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Bangap opening in metallic carbon nanotubes due to silicon impurities BRANDEN KAPPES, CRISTIAN CIOBANU, Colorado School of Mines — Controlling the bandgap of carbon nanostructures is key to the development and mainstream applications of carbon-based nanoelectronic devices. We report density functional theory calculations of the effect of silicon impurities on the electronic properties of carbon nanotubes (CNTs). We have found that silicon adatoms can open up a bandgap in intrinsically metallic CNTs. Even when the linear density of Si atoms is low enough that they do not create a bonded adatom chain, the bandgap opened in metallic CNTs can range between 0.10 eV and 0.47 eV, depending on adsorption site, linear density of Si atoms, and on the chirality of the nanotube.

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