The evolution of electronic and magnetic states for transition-metal rings embedded in carbon nanotubes

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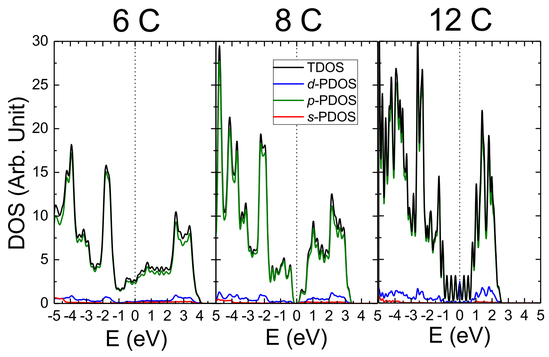
ABSTRACT:
We investigate the electronic and magnetic states for various sizes of transition metal rings that have been substituted into carbon nanotubes. Using density functional theory, we examine the electronic density of states, magnetic moment, and total energy for various transition metal atoms and magnetic configurations. After determining the structural and magnetic ground states, we show how the introduction of these metal atoms affect the electronic states and determine the ground state magnetic configuration with variation of transition metal atom and onsite potential. Future work will look into the use of these magnetic systems in a device application setting as we work towards a possible spintronic applications.

METHODS:
The *ab-initio* calculations are performed based on the density functional theory by using the atomistic orbital approach implemented in Atomistix Toolkit. Calculations are carried out within the spin-polarized generalized gradient approximation to the exchange-correlation functional (SGGA).

CONCLUSIONS:
The addition of transition-metal rings in carbon nanotubes produces magnetic-metallic behavior, which could lead to a possible control of the magnetic order with applied bias. Futures studies will evaluate this possibility.



The introduction of transition-metal atoms affects the overall electronic states and produces variable magnetic ground states

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