Computational studies of electronic and thermal properties of low dimensional materials

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THESEN ZUR DISSERTATION

1. Strategies to improve transport properties in nanomaterials

Downsizing materials to the nanoscale has been proved to improve their electronic, thermal and thermoelectric properties compared with their bulk counterpart. [1] Besides the advantages that implementation of low-dimensional systems can provide, additional strategies to enhance their performance, even beyond that point, are of interest to study.

2. Induced magnetism in phosphorene through chemical functionalization

Phosphorene, a 2D material without intrinsic magnetism, acquire local magnetic moment after chemical functionalization. The origin of the magnetization comes from the formation of a dangling bond after the rupture of the P-P bond, where one of the phosphorus atoms acts as the functionalization site and the other remains with the dangling electron.

3. Manipulation of electronic and magnetic properties of phosphorene

By modifying the lattice functionalization direction and the degree of functionalization coverage, the electronic band structure, magnetic ground state and total magnetization of the system can be manipulated. Several parameters of the electronic band structure, such as bandgap energy and direction and in-gap degeneration, can be modulated with the molecular arrangement and coverage of the functionalized molecules. The total magnetization was found to be proportional to the number of functionalized molecules in phosphorene, even though this trend is expected to fall after crossing a threshold.

4. Potential application of functionalized phosphorene systems as BMS

Phosphorene functionalized systems can be engineered to design bipolar magnetic semiconductors (BMS), which are a class of spintronic devices that can manipulate the electronic spin by controlling an electric voltage. Either by modulating the lattice direction, coverage or molecule type selection, the parameters that characterize the BMS have been proved to be enhanced.

5. Structural properties of phosphorene grain boundary systems under uniaxial strain

Grain boundaries is a type of defect that is common to find in nature, as a result of the merging of two crystals growing along different lattice directions. The emergence of this intersection changes the properties compared with its pristine counterpart. The starting point to analyze and understand the correlation between the grain boundaries and the deviation of their properties lies on the structural analysis around the grain boundary. The structural analysis in phosphorene grain boundaries under uniaxial strain shows that there is a dependence of the grain boundary type and the stretch-ratio off the in-plane or out-of-plane bonds. [2]

6. Electronic and thermal response of phosphorene grain boundaries under strain

The electronic and thermal properties of phosphorene is affected by the introduction of grain boundaries and strain. The grain boundary formation increases the electronic bandgap, in a different magnitude for each grain boundary type, but the applied strain gradually decreases the gap. Moreover, the thermal transmission is affect by the grain boundary, either in the whole spectrum or a region of the frequency spectrum, which is then larger affected with the strain.

7. Thermoelectric performance of phosphorene grain boundary systems

Pristine phosphorene is an anisotropic material, meaning that it exhibits different properties depending on the lattice direction. The thermoelectric performance of phosphorene along the armchair direction is better than along the zigzag direction. Even though the grain boundary and applied strain for the system along the zigzag direction showed a larger enhancement that the corresponding for the armchair direction, the thermoelectric performance of the second system remained with a better outcome, being the thermal conductance of the first system the main drawback for the development of thermoelectric devices.

8. Structural modification of CNT after fullerene encapsulation

Carbon nanotubes (CNT) peapods are a hybrid structure where fullerene molecules are encapsulated in a periodic array along the inner cavity of a CNT. Their properties vary depending on the interaction between the atoms of the CNT and the fullerenes. Experimental studies displayed an enhancement in the thermoelectric properties, but a full understanding of the cause was still unclear. [3] Computational simulations carried with DFTB of a CNT(8,8)@C_{60} showed that the CNT structure is distorted by the presence of the fullerenes, forming a periodic buckling along the CNT. This structural deformation decreases when the CNT diameter increases. [4]

9. Underlaying cause of electronic and thermal transmission variation in CNT peapods

A strong modification of the low-energy electronic conductance is caused by the presence of fullerenes, where the distance between CNT-C_{60} and C_{60}-C_{60} play a role in this outcome, demonstrating both conductance suppression and conductance enhancement compared with pristine CNT. In regard to the thermal transmission, a suppression at low and high frequencies modes is caused by the hybridization of local C60-derived modes with acoustic modes and also form the periodic buckling along the CNT surface.

10. Enhancing thermoelectric performance of CNT through fullerene encapsulation

The enhanced energy windows in the electronic transmission spectrum and overall suppression of thermal transmission in the CNT peapod increases their thermoelectric performance compared with its pristine CNT form by a factor of 2.2.

References

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