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Modeling of Diameter-Dependent Fe and Co Ultrathin Nanowires from First-Principles Calculations

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We present the electronic, magnetic, thermoelectric and optical properties of ferromagnetic metal nanowires (NWs) made of iron (Fe) and cobalt (Co) atoms using a first principles approach. Each property has been investigated as a function of atomic arrangement and nanowire diameter. Magnetic anisotropy is predicted originating from the spin–orbit coupling. Significant delocalization of electronic charge density is found in Fe nanowires with the increase in nanowire diameter, while the charge distribution anisotropy manifests in all the studied nanowire configurations. The thermoelectric properties exhibit strong coupling to the nanowire configuration and diameter. Thermal conductivity shows large divergence from the bulk iron and cobalt. The optical properties show the strongest increase for nanowires with large diameters. The theoretical modeling of configuration- and diameter-dependent nanowire properties serves as a cornerstone for future utilization of nanowire films in a variety of applications.

Biography:

Mr. Shivam Kansara working on low dimensional and multi-layered structure of transition metal in the framework of density functional theory using QE and VASP code. Mainly focusing on electronic, vibrational and transport properties to design new catalysts from transition metals

Aiming on the dynamical stabilities of the d block ultrathin nanowire to establish in nanodevices using Density Functional Perturbation Theory

In previous work [DOI: 10.1039/C7CP02072D], calculated the thermoelectric and optical properties of Fe and Co NWs using modelling of diameters. As well as, calculated the dynamically stable ultrathin nanowires of Pd and Pt NWs, which manuscript is under preparation for the 2D materials, he symmetrically investigated changes in electronic properties and phonon structures using induce strain [Computational Materials Science 141 (2018) 235–242] of dichalcogenides monolayers. The DFPT electron-phonon interaction is naturally screened as it is computed from the derivative of t