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TITLE:

ENHANCEMENT OF ELECTRON-PHONON COUPLING IN alkali-DOPED GRAPHENE AND THIN MgB_2 LAYERS

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ABSTRACT (250 words):

We present first principle investigation of enhancement of the electron-phonon coupling of superconducting alkali-doped graphene (e.g. LiC_6-mono) and thin layers of MgB_2 using density functional theory (DFT). These systems resemble in many ways, not only in geometry but as well as in electronic structure. Namely, like in alkali-C_6, where we have carbon hexagons with alkali adatom in the hollow site, in MgB_2 there are boron hexagons with Mg in hollow site.

For instance, both theoretical and experimental studies of LiC_6-mono proved a possibility of superconductivity in doped graphene. Continuing this investigation, we explored an enhancement of electron-phonon coupling and the raise of critical temperature in LiC_6-mono.

Inspired by similarity of intercalated graphite with MgB_2, we studied the electron-phonon coupling in MgB2 thin films. We used ab-initio calculations of phonon dispersion and electron-phonon-coupling within framework of DFT using Quantum Espresso. Our research included dopant and strain effects on an enhancement of electron-phonon coupling. We demonstrated an increase of electron-phonon coupling and critical temperatures.