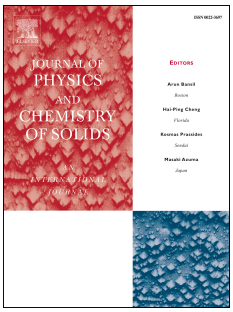
Accepted Manuscript



Metallization and superconductivity in Ca-intercalated bilayer MoS_2

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PII: S0022-3697(17)30907-1

DOI: 10.1016/j.jpcs.2017.08.003

Reference: PCS 8157

To appear in: *Journal of Physics and Chemistry of Solids*

Received Date: 23 May 2017

Revised Date: 18 July 2017

Accepted Date: 2 August 2017

Please cite this article as: R. Szczęśniak, A.P. Durajski, M.W. Jarosik, Metallization and superconductivity in Ca-intercalated bilayer MoS_2, *Journal of Physics and Chemistry of Solids* (2017), doi: 10.1016/j.jpcs.2017.08.003.

Metallization and superconductivity in Ca-intercalated bilayer MoS_2

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A two-dimensional molybdenum disulfide (MoS_2) has attracted significant interest recently due to its outstanding physical, chemical and optoelectronic properties. In this paper, using the first-principles calculations, the dynamical stability, electronic structure and superconducting properties of Ca-intercalated bilayer MoS_2 are investigated. The calculated electron-phonon coupling constant implies that the stable form of investigated system is a strong-coupling superconductor ($\lambda = 1.05$) with a low value of critical temperature ($T_C = 13.3$ K). Moreover, results obtained within the framework of the isotropic Migdal-Eliashberg formalism proved that Ca-intercalated bilayer MoS_2 exhibits behavior that goes beyond the scope of the conventional BCS theory.

Keywords: Superconductivity, First-principles study, Electron-phonon interaction, MoS_2

PACS numbers: 74.20.Fg, 74.25.Bt, 74.62.Fj

I. INTRODUCTION

The monolayer molybdenum disulfide (MoS_2) is a member of transitional metal dichalcogenides 2D materials family, with a stable hexagonal structure, analogous to that of graphene [1, 2]. The single-layer of MoS_2 consists of one monoatomic Mo plane placed between two monoatomic S planes in a trigonal prismatic arrangement which are bonded together through weak van der Waals interactions [3]. This layered structure has been one of the most interesting materials for scientists and engineers since it can exhibit often extraordinary outstanding electronic, thermal and optical properties [4–6]. For example, unlike the graphene, which does not have a band gap, single layer of MoS_2 is a semiconductor with a direct band gap of 1.90 eV [7, 8]. Interestingly, if we increasing the number of layers and thus the dimensionality from two (2D) to three (3D), MoS_2 becomes a semiconductor with an indirect band gap of about 1.29 eV [9, 10]. As a consequence of this feature, MoS_2 is expected to have a great potential for many practical applications, particularly in the next generation of nanoelectronic, optoelectronic and photoelectronic devices [11–14]. Also the superconducting properties of MoS_2 have been a target of intensive studies [15–19] since the discovery of graphene [1] and its metal-intercalated forms [20–23].

Intercalation is a well known method to getting new fascinating properties that are usually distinctly different from those observed in the pristine materials. For example, a zero-gap semimetal graphene, can be transformed into a metallic, superconducting, semiconducting or insulating state by either physical or chemical modification [24–26]. Very recently, a few studies reported the observation of superconductivity in Ca-intercalated bilayer graphene with the onset tempetarure of 4 K [27], Ca-doped graphene laminates around 6.4 K [28] and Li-decorated monolayer graphene at 5.9 K [29].

Inspired by the recent success in determining the superconducting state in Li- and Na-intercalated bilayer MoS_2 [15, 16] in the present paper we decided to examine the dynamical stability and superconductivity of Ca-intercalated bilayer molybdenum disulfide $(MoS_2)_2Ca$.

II. COMPUTATIONAL DETAILS

The electronic and phonon structures of Ca-intercalated bilayer MoS_2 have been studied by *ab-initio* calculations based on the density functional theory (DFT) using the PWscf program of the Quantum-ESPRESSO package [30, 31]. The ultrasoft pseudopotentials for Mo, S and Ca atoms, and the generalized gradient approximation according to the Perdew-Wang 91 gradient-corrected functional were employed for atom-atom interactions in phonon dispersion determinations and electron-atom interactions in electron-phonon coupling calculations. After performing convergence tests, a plane-wave energy cutoff of 80 Ry is used. In order to simulate the 2D system, we use periodic boundary condition with a vacuum space of 20 Å along the non-periodic z direction. For electronic calculations, the Brillouin zone (BZ) is sampled in a $30 \times 30 \times 1$ Monkhorst-Pack k-mesh with gaussian smearing of 0.01 Ry. To calculate the electron-phonon coupling matrix and the phonon spectrum, a k-mesh of $60 \times 60 \times 1$ and a q-mesh of $6 \times 6 \times 1$ are used. We performed total energy calculations for a series of the lattice parameters. For each lattice parameter the atomic positions were relaxed according to the atomic forces. This procedure was repeated until the forces on every atom of the unit cell was less than 0.002 Ry/a.u. In this way, the fully relaxed structural parameters of $(MoS_2)_2Ca$ have been obtained.

III. RESULTS AND DISCUSSION

In the pristine monolayer MoS_2, a hexagonal molybdenum atoms plane is sandwiched between two hexagonal

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