全国大学英语四级考试
成绩报告单

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笔　试

准考证号：372510172120025
考试时间：2017年12月

总分	听力 (35%)	阅读 (35%)	写作和翻译 (30%)
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教育部考试中心
证书专用章

西南林业大学研究生成绩单

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入学年月	2020-09-23		毕业年月		2023-12-15	学制	3

类别	课程名称	学时数	学分	开课学期	成绩	备注
学位课	自然辩证法概论		1.0	1	88.00	
	专业英语		2.0	1	84.00	
	矩阵分析与计算方法		3.0	1	75.00	
	英语听力		0.5	1	71.00	
	先进制造技术		2.0	2	70.00	
	英语口语		0.0	1	76.00	
	英语精读		1.5	1	71.00	
	现代控制理论		2.0	1	91.00	
	英语精读		1.5	2	62.00	
	英语写作		0.0	2	67.00	
	学位英语		0.0	2	64.00	
	英语听力		0.5	2	62.00	
	中国特色社会主义理论与实践研究		2.0	2	80.00	
	信号分析与数据处理		2.0	2	78.00	
	学位课小计		18.0			
非学位课	汽车动力学		2.0	1	70.00	
	弹性力学及有限元		2.0	2	73.00	
	机电一体化		2.0	2	82.00	
	机械优化理论		2.0	2	85.00	
	非学位课小计		8.0			

学位（毕业）论文题目	新型高性能二维碳基储能材料的研究		
论文答辩时间	2023-12-08	论文答辩成绩	76
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学院（部）（盖章）
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ORIGINAL ARTICLE

QHOD-Net: A New Highly Metallic Two-Dimensional Carbon Allotrope Material

Detong Kong[1] · Lihui Zhong[2] · Chengling Wu[3] · Xiao Wang[3] · Zhentao Yuan[3] · Xingrui Zheng[3] · Yuan Wang[1]

Received: 26 July 2022 / Accepted: 26 September 2022

Abstract We propose a new two-dimensional metallic carbon allotrope named QHOD-net using first-principles calculations, the structure of which includes five carbon rings; quadrangular, pentagonal, hexagonal, octagonal, and decagonal. This metastable phase metallic carbon material displays anisotropic mechanical properties, and its smallest and largest in-plane stiffness have been calculated to be $C_a = 261$ GPa nm and $C_b = 240$ GPa nm, respectively, both much lower than for graphene. The Poisson's ratio is as low as 0.29, which has good toughness. The DFT indicates that QHOD-net is metallic with no bandgap in the entire BZ region and one band crosses the Fermi level. At the Fermi level, the electron density of states per atom is much higher, reaching ~ 0.297 eV/states/per atom. In addition, we have performed the 3D stacked structure of the two-dimensional structure QHOD-net, and the results of our study indicate that the stacked structure is a super-hard 3D carbon material (74.8 GPa nm). The two-dimensional structure QHOD-net contains a large number of tetragonal, pentagonal, octagonal, and decagonal carbon rings than the perfect hexagonal shape of ideal graphene. The disorder of the material is increased compared to that of graphene. It is this disorder that triggers these interesting findings, and in addition we provide a new strategy for the design of 2D structures with multiple carbon rings.

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1 Introduction

Due to the rich electronic hybridization configurations of *sp, sp*^{2}, and *sp*^{3} orbitals, carbon is the most versatile element and able to form many allotropes, of which zero-dimensional fullerenes [1], one-dimensional carbon nanotubes [2], and two-dimensional (2D) graphene [3] are the three most typical examples. Among them, the unique 2D inorganic honeycomb structure and the fascinating physical properties of graphene have greatly motivated researchers to explore new 2D carbon materials [4–7]. Many allotropes of carbon with peculiar properties have been discovered, such as penta-graphene [8], which has a negative Poisson's ratio and ultra-high ideal strength. Furthermore, 2D carbon allotropes such as QPHT-graphene [9], h567 [10], net-τ [11], Kust-I [12], Thgraphene [13], and Bp-sheet 5 [14] have been predicted. These new carbon allotropes exhibit various electronic properties ranging from metals to semimetals and semiconductors [15].

The biphenylene network (BPN) [16], a fully sp2-hybridized carbon allotrope with a planar structure, has recently been successfully synthesized in an experiment. In addition, theoretical predictions of the 2D M-C crystals [17] can also be made using the already synthesized structure γ-graphyne [18]. This has greatly promoted theoretical prediction studies of 2D carbon allotropes. Based on previous research, researchers have been able to achieve the construction of 2D graphene allotropes in two ways. The first approach is to obtain 2D carbon allotropes by exfoliating them from known materials, such as penta-graphene from T12 carbon [19].

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Full Length Article

Novel two-dimensional C_6B_4 monolayer as an anode for Li-/Na-ion batteries with high theoretical capacity

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ABSTRACT

In this study, we predict a two-dimensional (2D) multi-ring structure composed of carbon and boron atoms by first-principles calculations, and investigate its potential for lithium/sodium storage. The cells in this structure are composed of six carbon and four boron atoms (hence the name *k*-C_6B_4). Its stability as well as mechanical, electronic, and energy storage-related properties are also investigated. The results show that *k*-C_6B_4 has a high density of states of 0.328 states/eV/atom at the Fermi level, with maximum values of the Young's modulus and Poisson's ratio of 272.39 N/m and 0.4, respectively. This shows that *k*-C_6B_4 has good electrical conductivity and mechanical ductility such that it can avoid damage during the charging and discharging processes. Moreover, the barriers to the diffusion potential of *k*-C_6B_4 for the Li and Na ion were 0.195 eV and 0.123 eV, respectively, which are important for efficient charging and discharging. Most importantly, *k*-C_6B_4 has a high specific capacity of 1395 $mAhg^{-1}$ for Li/Na ions. These findings suggest that the 2D *k*-C_6B_4 is a promising anode material for LIBs/NIBs, and provides a new strategy for energy storage.

1. Introduction

The increasing global demand for energy is driving the development of energy storage devices with a higher energy density. Lithium-ion batteries have played an important role in this context due to their portability and long cycle life [1,2]. Despite their considerable success, however, the high cost, scarcity, and low specific capacity of lithium make it unsuitable for completely satisfying the demand for energy storage [3,4]. Sodium has been considered as an alternative because its chemical properties are similar to those of lithium. Sodium is cheap, non-toxic, and abundant in nature [5,6]. It is also much safer use in batteries with compared with lithium [7]. Therefore, developing high-performance electrodes for NIBs is important.

Considerable effort has been devoted to exploiting novel electrode materials for LIBs/NIBs over the last few decades [8–11]. Two-dimensional (2D) materials have unique physical properties and large surface areas, because of which they have been investigated in this domain. Increasing numbers of 2D materials are being discovered and used, including graphene, boropnene, and phosphorene [12–14]. However, most 2D anode materials used thus far do not address the problem of the structural stability of the material and the formation of Li/Na dendrites during energy storage, which in turn leads to a significant reduction in their energy storage capacity.

Research on high-density energy storage has generally followed two directions: The first is to construct ordered macrocycles of graphene. However, the structure of such materials is affected by the bond length such that their capacity for energy storage is limited [15,16]. The second direction of research involves identifying point defects on 2D diluted silicon or graphene [17–19]. However, the material fails to maintain its original structure during charging and discharging in this case, and is prone to structural failure. Atomic substitution can be carried out in such two-dimensional materials as B, P, and Ta [20–22] so that the substituted structures have sp^2 hybridization and a high capacity for energy storage.

In this study, we have predicted a stable 2D material called *k*-C_6B_4. We perform first-principles calculations of its structure, and the results show that *k*-C_6B_4 is stable, and has a high electrical conductivity and excellent mechanical properties. Both sodium and lithium atoms have a low potential barrier for diffusion and a high specific capacity. Therefore, the 2D material based on *k*-C_6B_4 offers potential for use as a high-

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Metal (Au, Ag, Pt) Doping Effects on the Gas-Sensing Mechanism and Characteristics of Two-Dimensional WS_2: A First-Principle

Detong Kong,[§] Beibei Ma,[§] Ling Zhang,* Lei Yang, Chao Li, Chengbin Yin, Keyang Wu, and Yuan Wang*

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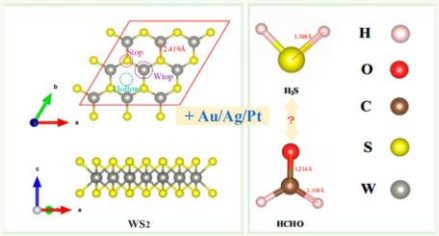
ABSTRACT: Highly sensitive gas sensors play a crucial role in monitoring the concentration of harmful gases within automobile interiors, ensuring the well-being of occupants. In this study, a computational approach employing density-functional theory was utilized to investigate the gas-sensing performance of two-dimensional WS_2 nanomaterials doped with precious metals (Au, Ag, and Pt), particularly in the detection of hazardous gases such as formaldehyde (HCHO) and hydrogen sulfide (H_2S). The research findings indicate that the introduction of precious metal dopants significantly enhances the sensitivity of WS_2 to both H_2S and HCHO gases, concurrently improving the material's electronic properties and stability. Furthermore, metal doping into the WS_2 system induces a more pronounced electron transfer during the adsorption process with target gases, thereby further augmenting the intrinsic sensitivity of WS_2 to the target gases. Considering the desorption performance of gases, Ag−WS_2 emerges as a promising candidate for detecting HCHO and H_2S at room temperature. Au−WS_2, which is stable in adsorbing HCHO at room temperature and rapidly desorbing at elevated temperatures, presents itself as a potential material for efficient and reusable HCHO sensing at high temperatures. These research findings provide unique insights and directions for the development of efficient and sensitive gas sensors, offering robust support for addressing issues related to environmental monitoring. By delving into the gas-sensing performance of two-dimensional WS_2 nanomaterials under different metal dopings, this study contributes valuable references for the design of innovative sensor materials and technologies.



KEYWORDS: *two-dimensional material, WS_2, gas analysis, gas sensor, density-functional theory*

INTRODUCTION

In recent years, with the increasing ubiquity of automobiles, the issue of air quality within the vehicle cabin has garnered significant attention.[1] The harmful gases present in the car interior primarily stem from the oxidative release of interior materials, resulting in the generation of formaldehyde (HCHO) and incomplete combustion-produced hydrogen sulfide (H_2S). These gases pose severe health risks to individuals.[2−4] Furthermore, due to the typically confined and relatively enclosed driving space within the vehicle cabin, harmful gases struggle to disperse rapidly. Once the concentration of harmful gases within the vehicle surpasses a certain threshold, it poses a substantial risk to people's health.[5,6] Therefore, there is an urgent need for a high-precision, real-time gas detection method to proactively identify gas components, monitor harmful gas concentrations, and adapt to various environmental conditions.

Two-dimensional transition metal dichalcogenides (TMDs) have garnered significant attention due to their graphene-like layered structure.[7−10] This endows them with outstanding electrical,[11] chemical,[12] mechanical,[13] and optical[14] properties. Consequently, 2D TMDs are widely regarded as having enormous potential for applications in the sensor field. Among them, two-dimensional tungsten disulfide (WS_2), with its folded hexagonal structure, exhibits extensive prospects in the field of gas sensing owing to its unique crystal structure and physicochemical properties, such as high charge carrier mobility,[15] tunable band gap,[16] and high specific surface area.[17] While WS_2 was initially employed primarily as a lubricant in the past, its increasing prominence in electronic devices has become evident with deeper research.

Tang et al. have predicted through first-principles studies that the vertical stacked heterostructure (V-MoS_2−WS_2)

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