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Adopting Big Data to Accelerate Discovery of 2D TMDCs Materials via CVR Method for the Potential Application in Urban Airborne Hg^0 Sensor

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Abstract

Airborne Hg^0 has significant negative effect on cities and urban systems. The development of effect airborne Hg^0 sensor is rather important for both urban atmospheric Hg^0 detection and the evaluation of Hg^0 capture materials. Previous research showed MoS_2 as a typical TMDCs materials had excellent performance to capture Hg^0. In this study, the other 2D TMDCs materials via CVR method in big data was initially studied for the potential urban airborne Hg^0 sensor application. The combinations of Pymatgen initial screening, Factsage thermochemical screening and Aflow structural screening were developed for accelerating discovery of the 2D TMDCs in big data. The results from Pymatgen showed that except elements Cd, Sc, Y, Zn, and the other elements have the potential to form TMDC. Furthermore, elements such as Co, Ni, Mo, Ru, W and Ir have the ability forming pure TMDC and Ti, Mn, Zr and Pd can only form partial TMDC. However, other elements such as Sc, V, Cr, Fe, Cu, Zn, Y, Rh and Cd have no possibility to form TMDC. Finally, TiS_2, NiS_2, ZrS_2, MoS_2, PdS_2 and WS_2 were found with 2D structure, which are possible to be prepared by the S-CVR method as the airborne Hg^0 sensor materials.

Selection and peer-review under responsibility of the scientific committee of the CUE2018-Applied Energy Symposium and Forum 2018: Low carbon cities and urban energy systems.

Keywords: 2D TMDCs Materials; Hg^0 Sensor, urban atmospheric Hg^0 detection; Big Data Screening

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1. Introduction

Mercury is harmful to ecosystem and human health for its toxicity, bio-accumulation characteristics and persistence in environment[1]. In particularly, elemental mercury (Hg^0) is in gaseous form and is volatile, and because of the long residence time, transported over long distances[2]. It has the significant negative effect on both locally and globally environment, especially cities and urban systems. It was demonstrated that the significant impact of the Chicago/Gary urban area on atmospheric Hg concentrations across the whole Lake Michigan Basin. A study showed that mercury emission had the evidences of rural-to-urban migrants in Beijing, China in recent years[3].

Recently, an international treaty called Minamata Convention has been ratified by 90 countries, which is introduced to control anthropogenic mercury emission that had come into effect in 2017[3]. Hence, there have been considerable interests worldwide in the development of mercury monitoring devices and mercury capture materials with equipment. Therefore, the effect airborne Hg^0 sensor is important for both urban atmospheric Hg^0 detection and the evaluation of Hg^0 capture materials.

The promising 2D material grapheme is triggered attention due to its unique chemical and physical properties[4-6]. Apart from the graphene, the graphene-like material strengthens the application capability within the more flexible, diversiform and functional properties, therefore, the graphene-like material as alternative of graphene has dramatically used for a wide range[7-10]. Transition-metal dichalcogenides (TMDCs) is a kind of two-dimensional (2D) graphene derivative material, which fundamentally is stacked vertically like a sandwich, which two layer of chalcogen atom connects with the transition metal, and layered weakly in the horizontal direction due to the interaction of the van der Waals forces[7, 11, 12].The monolayer molybdenum disulfide (MoS_2) is a typical substance of TMDCs, which frequently applies in electronchemical region [13, 14]. According to the active chemical, physical and electronic properties, TMDCs have widely potential application in term of the following region[15], the electrochemical domains, energy conversion energy conversion technology, lithium ion battery application for energy storage device[16-18], drug delivery monitoring[8], desulfurization catalyst[19], mercury absorbent[1, 20-24]. Hence, there is a great potential that the 2D TMDCs Materials to be applied in the development of urban airborne Hg^0 sensor.

It is quite significant to prepare TMDCs within a governable method in term of the potential application[25], which can be divided into two general kind, the top-down method and bottom-up approach, respectively[26]. The top-down method, liquid-phase exfoliation(LPE), breaks the van der Waals forces in the horizontal layer in the solvent[27], however, its defects existed on many aspects, it requests the flake dimension, removes the solvent after fabrication, furthermore, although it satisfies to apply on the catalysis and sensor, it also needs to improve for electrochemical domains[6]. On the other hand, the bottom-up method, chemical vapor deposition (CVD) or chemical vapor reaction (CVR) are relievable methods to manufacture monolayer TMDCs, which control the layers and edge structure, comparing to the LPE [9, 28]. Furthermore, dramatic development of the TMDCs cause the massive demand in available application, the low cost and high quantity is a rough challenge for TMDCs product, the process of CVD/CVR growth of TMDC can solve this problem in some degree[12, 29]. MoS_2 as the famous representative of TMDCs, the detail of preparation of MoS_2 is that the oxide of molybdenum supplies the transition metal (Mo) reacts with the vapor gas hydrogen sulfide to work the mechanism of deoxygenation within adding hydrogen continuously. The hydrogen plays an significant role in the reaction, not only as the catalysis to accelerate the reaction, but also control the atomic ratio of Mo and S to prevent to work oxidation[30].

The hydrogen, hydrogen sulfide, molybdenum disulfide（MoS_2）in the condition of specific temperature approximately 400 ^{0}C can form various and different percentage product, therefore, it controls the partial fraction is curial factor to obtain the final product.[30] Apart from MoS_2, other transition metal oxidate react with hydrogen sulfide, which can be investigated whether it can form the specific TMDC. Therefore, previously, the investigation of prediction of the final output can be achieved by the machine model technique (ML) in big data[31]. Based on the hypothetical theory, the ML can simulate the tens of thousands of quantitative results, no matter the success or fail to gain the ideal product; the results from the ML can provide the useful information. For an instance, the identified transition metal can form TMDC at the proper temperature by CVR. The method of ML makes the great process to collect the massive results and settle regularly to set up a standard database, then the experiment can approve the result according to the database and make the consideration of the real situation to achieve the technique visible[32]. Therefore, the aim of this study is to initially study the 2D TMDCs materials via CVR method in big data for the potential urban airborne Hg^0 sensor application.

2. Methodology

2.1 Pymatgen

The Python Materials Genomics (pymatgen) library, a robust, is an open-source Python library for materials analysis[33]. A key enabler in high-throughput computational materials science efforts is a robust set of software tools to perform initial setup for calculations and post-calculation analysis to derive useful material properties from raw calculated data. The pymatgen library is written by the Python programming language, and leverages the large number of available standard and scientific programming libraries. The library is basically related to the object-oriented programming paradigm to facilitate code reuse and ensure modularity in design.

In our study, we used this software to generate three phase diagram with three different substance in order to show its product with different content by import our code needed and elements into pymatgen. Then the software will operate and display three phase diagram we required automatically. Several articles have demonstrated that elements Mo and W can form TMDC, which is not only relatively simple to form but have the 2-Dimonsions structure. In our experiment, we are willing to find whether a wider district of transition metal area in periodic table of the elements have the potential forming TMDC or part of them, which need enormous experiment and a great amount of time. Therefore, modeling experiment based on databases is a suitable alternative method to determine the product of transition mental elements in H_2S/H_2 environment through S-CVR method at 400℃.

To confirm whether these elements can form TMDC at a certain temperature to fit chemical vapor deposition and whether these elements can form pure TMDC or form TMDC with other compounds. Pymategen is a suitable database to confirm the potential of forming TMDC of an element. In Pymatgen, elements can be determined the products that can form with other 3 elements. In this case, we can decline the number of elements that we should concern if some elements cannot form TMDC at any condition. However, to ensure the preciseness of the databases, all the first three rows of transition metal elements are taken into consideration in next steps. The elements can be acquired from medicine containing this certain element. CVR method requires a solution environment; hence, the elements are chosen as soluble medicine from Aladdin Co. Ltd. To ensure there is no disturb compound generate, the medicine is selected only contain the require element and nitrate/ammonium. We can then obtain the stable oxidation for the medicine and then the condition for these transition elements forming TMDC.

2.2 FactSage

FactSage is a commercial thermochemical software and database package. In our project, FactSage is used to form phase diagram. There are two steps need this software: one is determined the which stable compound will form from medicine acquired from Aladdin co. ltd. To fit CVR method, the temperature is set 520℃ and the medicine is calcinated in air. Hence, the three elements in phase diagram are set as medicine, N_2, and O_2 at 520℃. In this type of diagram, we can determine whether this medicine can form stable oxidation that can be used in the next step. Another step is determined the compounds that will form with CVR method. From former literature data, the most proper environment forming TMDC is 400℃, $H_2S(g)$ in H_2[19]. Therefore, the three elements in phase diagram are set as stable oxidation, H_2S and H_2 at 400℃. In this type of diagrams, we can determine whether the element can form pure TMDC at a certain composition or partial TMDC with other compounds at a certain composition or cannot form TMDC.

2.3 Aflow

Aflow comprising phase-diagrams, electronic structure and magnetic properties, generated for high-throughput calculations of materials properties[15]. This continuously updated compilation currently contains over 150,000 thermodynamic entries for alloys, covering the entire composition range of more than 650 binary systems, 13,000 electronic structure analyses of inorganic compounds, and 50,000 entries for novel potential magnetic and spintronics systems. The repository is available for the scientific community on the website of the materials research consortium, aflowlib.org.

Aflow is a library that concludes a great number of crystalline information, in this study, the Aflow is used to get the structure of the studied samples. The aspect of the figure of crystalline structure are chose to straightly evaluate the 2D structures.

3. Results & Discussions

3.1 Pymatgen initial screening

The line in Pymatgen is the convex hull line. The distance between the line and the phase is the energy that forming this compound. The red points on the hull line, which means the energy forming this compound is zero, indicate that the compound should be a stable phase, meaning it can be produced relatively simply in theory.

The results from Pymatgen shows that except elements Cd, Sc, Y, Zn, and the other elements have the potential to form TMDC. The examples of the Mo and Cd elements are illustrated in Fig. 1.

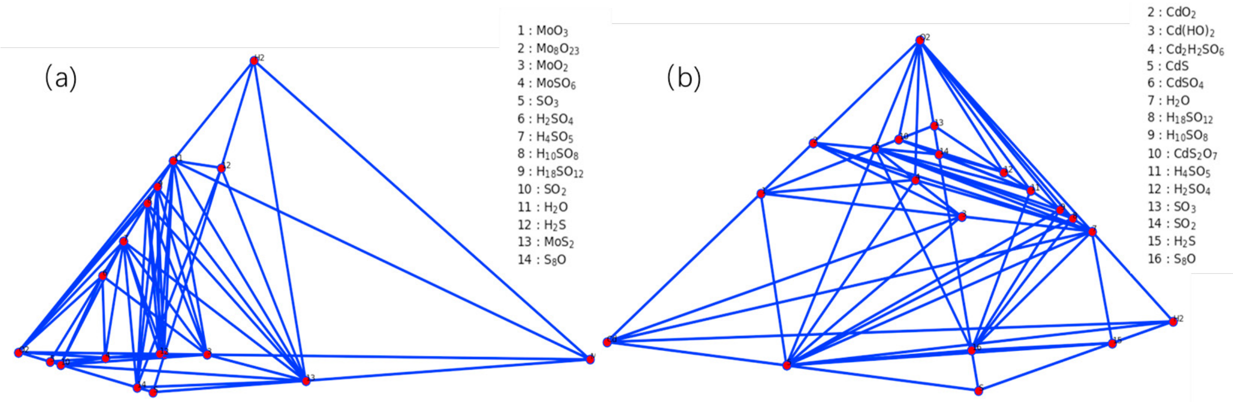

Fig. 1. The examples of the Mo element (a) has the potential to form TMDC and Cd element (b) cannot form TMDC

3.2 Factsage thermochemical screening

For the precursors, elements Nb, Tc, Hf, Ta and Re cannot find a soluble source from Aladdin Co. Ltd. Elements Ag, Pt and Au form elementary substance at 400°C. These elements in a heat environment have the tendency to form stable elementary substance. The data of elements Os and Hg are lacking in FactSage. Hence, these elements are not possible to do thermochemical screening. The possible precursors were calculated by Factsage with phase diagram model and the oxidation products are listed in Table 1. The screened oxidation products will be the candidates for further CVR study.

Table 1. Oxidation products from precursors.

	IIIB	IVB	VB	VIB	VIIB	VIII			IB	IIB
4	Sc_2O_3	TiO_2	V_2O_5	Cr_2O_3	Mn_2O_3	Fe_2O_3	Co_3O_4	NiO	CuO	ZnO
5	Y_2O_3	ZrO_2		MoO_3		RuO_2	RhO_2	PdO_2	Ag	CdO
6				WO_3			IrO_2	Pt	Au	

Table 2. Products of oxidation forming pure and partial TMDC (group 1) and forming partial TMDC only (group 2)

Group 1	I	II		Group 2	I	II
a	CoS_2	CoS_2+Co_9S_8+$CoSO_4$		a	TiS_2+TiO_2	TiO_2+Ti_2S_3
b	NiS_2	NiS_2+Ni_3S_4		b	MnS_2+MnS	MnS
c	MoS_2	MnO_2+MnS_2+Mn_4O_{11}		c	ZrS_2+ZrO_2	ZrS_3+ZrO_2
d	RuS_2	Ru+RuS_2		d	PdS_2+PdS	PdS
e	WS_2	WS_2+ WS_3				
f	IrS_2	IrS_2+Ir_2S_3				

For the elements that form stable oxidation, in the H_2S/H_2 environment, Co, Ni, Mo, Ru, W and Ir have the ability forming pure TMDC at specific area (Group 1 as shown in Table 2). They can also form partial TMDC with other compounds in some area. Elements Ti, Mn, Zr and Pd cannot form pure TMDC in all areas. However, they can form partial TMDC in some areas (Group 2 as shown in Table 2). Other elements forming stable oxidation, Sc, V, Cr, Fe, Cu, Zn, Y, Rh and Cd have no possibility forming TMDC. These elements are corresponding with the results from Pymatgen.

3.3 Aflow structural screening

Combining the previous section, there are 10 transition metals have potential to form TMDC within the method CVR. However, the filtration between the MX_2 should satisfy two conditions at the same time, which can be prepared by CVR and has the 2D layered structure. Therefore, the Aflow is used to investigate each MX_2' s 2D structure. The supercell of crystal can be adjusted to unify the top and side view of each structure, which is convenient to investigate the specific structure. As a result, TiS_2 NiS_2 ZrS_2 MoS_2 PdS_2 and WS_2 (as example shown in Fig. 2.(a)) are satisfied the 2D structure, which is indicated from the top view and side view structure. On the other hand, the other 4 crystal, although they can form TMDC within CVR, it is not the 2D layered structure. They are MnS_2 , CoS_2 ,RuS_2 and IrS_2 (as example shown in Fig. 2.(b)). By the structural screening with Aflow database, the 2D structures could be clearly identified as shown in the Fig. 2 (as the example due to the page limitation).

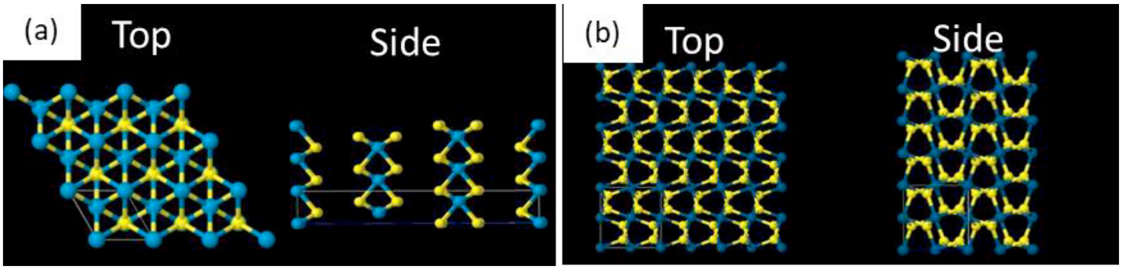

Fig. 2. The examples of the WS_2 (a) has the potential to form 2D TMDC and IrS_2 (b) cannot form 2D TMDC

4. Conclusion

For both urban atmospheric Hg^0 detection and the evaluation of Hg^0 capture materials, the development of effect airborne Hg^0 sensor is important. In this study, the other 2D TMDCs materials via CVR method in big data was initially studied for the potential urban airborne Hg^0 sensor application. The combinations of Pymatgen initial screening, Factsage thermochemical screening and Aflow structural screening were developed for accelerated discovery of the 2D TMDCs in big data. By Pymatgen initial screening, it was found that except elements Cd, Sc, Y, Zn, and the other elements have the potential to form TMDC. Furthermore, elements such as Co, Ni, Mo, Ru, W and Ir have the ability forming pure TMDC whilst elements such as Ti, Mn, Zr and Pd can only form partial TMDC. Finally, TiS_2, NiS_2, ZrS_2, MoS_2, PdS_2 and WS_2 were found with 2D structure by Aflow structural screening. Based on the results, it is possible that samples such as TiS_2, NiS_2, ZrS_2, MoS_2, PdS_2 and WS_2 can be prepared by the S-CVR method as the airborne Hg^0 sensor materials. The application results with different ability of various materials will be verified in the future study.

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References

[1] ZHAO H, MU X, YANG G, et al. Graphene-like MoS2 containing adsorbents for Hg0 capture at coal-fired power plants [J]. Applied Energy, 2017, 207(Supplement C): 254-64.

[2] NANSAI K, OGUCHI M, SUZUKI N, et al. High-Resolution Inventory of Japanese Anthropogenic Mercury Emissions [J]. Environmental Science & Technology, 2012, 46(9): 4933-40.
[3] RU M, TAO S, SMITH K, et al. Direct Energy Consumption Associated Emissions by Rural-to-Urban Migrants in Beijing [J]. Environmental Science & Technology, 2015, 49(22): 13708-15.
[4] GUO A-B, JIANG W, ZHANG N. Magnetic properties of a doped graphene-like bilayer [J]. Physica B: Condensed Matter, 2017, 513(21-8.
[5] DONG Y, WU Z-S, REN W, et al. Graphene: a promising 2D material for electrochemical energy storage [J]. Science Bulletin, 2017, 62(10): 724-40.
[6] VELICKý M, TOTH P S. From two-dimensional materials to their heterostructures: An electrochemist's perspective [J]. Applied Materials Today, 2017, 8(68-103.
[7] ZHU C, DU D, LIN Y. Graphene-like 2D nanomaterial-based biointerfaces for biosensing applications [J]. Biosens Bioelectron, 2017, 89(Pt 1): 43-55.
[8] TIAN F, LYU J, SHI J, et al. Graphene and graphene-like two-denominational materials based fluorescence resonance energy transfer (FRET) assays for biological applications [J]. Biosens Bioelectron, 2017, 89(Pt 1): 123-35.
[9] FU Q, XIANG B. Monolayer transition metal disulfide: Synthesis, characterization and applications [J]. Progress in Natural Science: Materials International, 2016, 26(3): 221-31.
[10] NIKAM R D, SONAWANE P A, SANKAR R, et al. Epitaxial growth of vertically stacked p-MoS2/n-MoS2 heterostructures by chemical vapor deposition for light emitting devices [J]. Nano Energy, 2017, 32(454-62.
[11] ARAB A, DAVYDOV A V, PAPACONSTANTOPOULOS D A, et al. Monolayer MoS2 Nanoribbons as a Promising Material for Both n-type and p-type Legs in Thermoelectric Generators [J]. Journal of Electronic Materials, 2016, 45(10): 5253-63.
[12] WONG S L, LIU H, CHI D. Recent progress in chemical vapor deposition growth of two-dimensional transition metal dichalcogenides [J]. Progress in Crystal Growth and Characterization of Materials, 2016, 62(3): 9-28.
[13] ZHAO H, MU X, YANG G, et al. Graphene-like MoS 2 containing adsorbents for Hg 0 capture at coal-fired power plants [J]. Applied Energy, 2017,
[14] HAO S, YANG B, GAO Y. Controllable growth and characterizations of hybrid spiral-like atomically thin molybdenum disulfide [J]. Physica E: Low-dimensional Systems and Nanostructures, 2016, 84(378-83.
[15] CURTAROLO S, SETYAWAN W, WANG S, et al. AFLOWLIB.ORG: A distributed materials properties repository from high-throughput ab initio calculations [J]. Computational Materials Science, 2012, 58(227-35.
[16] ZHANG G, LIU H, QU J, et al. Two-dimensional layered MoS2: rational design, properties and electrochemical applications [J]. Energy & Environmental Science, 2016, 9(4): 1190-209.
[17] LI Z, ZHANG L, LI B, et al. Convenient and large-scale synthesis of hollow graphene-like nanocages for electrochemical supercapacitor application [J]. Chemical Engineering Journal, 2017, 313(1242-50.
[18] DING W, XU L, CHEN X, et al. Large-Scale Fabrication of Graphene-like Carbon Nanospheres for Lithium Ion Battery Application [J]. Electrochimica Acta, 2016, 218(237-42.
[19] ZHAO H, LUO X, HE J, et al. Recovery of elemental sulphur via selective catalytic reduction of SO2 over sulphided CoMo/γ-Al2O3 catalysts [J]. Fuel, 2015, 147(67-75.
[20] ZHAO H, FAN H, YANG G, et al. Integrated Dynamic and Steady State Method and Its Application on the Screening of MoS2 Nanosheet-Containing Adsorbents for Hg0 Capture [J]. Energy & Fuels, 2018,
[21] ZHAO H, GANG Y, XIANG G, et al. Hg0-Temperature-Programmed Surface Reaction for the Study of a Suite of Metal Oxides and Mo-Promoted Metal Oxides for Hg0 Capture [J]. Fuel, 2016, A manuscript number has been assigned: JFUE-D-16-00240(
[22] ZHAO H, MU X, YANG G, et al. Microwave-induced activation of additional active edge sites on the MoS2 surface for enhanced Hg0 capture [J]. Applied Surface Science, 2017, 420(439-45.
[23] ZHAO H, YANG G, GAO X, et al. Hg0 capture over CoMoS/γ-Al2O3 with MoS2 nanosheets at low temperatures [J]. Environmental Science & Technology, 2015,
[24] ZHAO H, YANG G, PANG C H, et al. Screening of Metal Oxidesfor Hg 0 Capture [J]. Energy Procedia, 2015, 75(2421-6.
[25] BAI H, MA J, WANG F, et al. A controllable synthesis of uniform MoS 2 monolayers on annealed molybdenum foils [J]. Materials Letters, 2017, 204(35-8.
[26] YANG Y, PU H, LIN T, et al. Growth of monolayer MoS 2 films in a quasi-closed crucible encapsulated substrates by chemical vapor deposition [J]. Chemical Physics Letters, 2017, 679(181-4.
[27] LATE D J. Liquid exfoliation of black phosphorus nanosheets and its application as humidity sensor [J]. Microporous and Mesoporous Materials, 2016, 225(494-503.
[28] MAHYAVANSHI R D, KALITA G, SHARMA K P, et al. Synthesis of MoS 2 ribbons and their branched structures by chemical vapor deposition in sulfur-enriched environment [J]. Applied Surface Science, 2017, 409(396-402.
[29] SHIN Y C, DRESSELHAUS M S, KONG J. Preparation of Graphene with Large Area [J]. 2014, 39-76.
[30] LI X, LI X, ZANG X, et al. Role of hydrogen in the chemical vapor deposition growth of MoS2 atomic layers [J]. Nanoscale, 2015, 7(18): 8398-404.
[31] <machine-learning technique could revolutionize how materials science is done.pdf> [J].
[32] ISAYEV O, OSES C, TOHER C, et al. Universal fragment descriptors for predicting properties of inorganic crystals [J]. Nat Commun, 2017, 8(15679.
[33] ONG S P, RICHARDS W D, JAIN A, et al. Python Materials Genomics (pymatgen): A robust, open-source python library for materials analysis [J]. Computational Materials Science, 2013, 68(314-9.