Ab initio study of structural and mechanical properties of two-dimensional Mo_2ScC_2

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ABSTRACT

"MXene", a new class of two dimensional materials, has attracted considerable research interest due to its outstanding physical properties as well as promising technological applications. In this work, the structural, and mechanical properties of the Monolayer Mo_2ScC_2 compound is calculated first time within the framework of the density-functional theory (DFT) by using the plane-wave pseudopotential approach as implemented within the VASP package. The structural parameters of Mo_2ScC_2 is optimized, and calculated the lattice parameters. We think that the results will guide the experimental work that is not yet done.

1. INTRODUCTION

MAX phases constitute a class of nanolaminated ternary carbides and nitrides, described by the general formula, $M_{n+1}AX_n$ (n =1, 2, 3, etc) where M is a transition metal, A is an A–group element, and X is usually C or N. MAX phases adopt the hexagonal P63/mmc structure in which M and X atoms form octahedral edge-sharing building blocks interleaved by A-atomic layers. This structure is highly anisotropic and catalytic for the combination of metallic and ceramic characteristics in MAX phases [1].

MXenes are a new class of 2D transition metal carbides and nitrides with chemical formula of $M_{n+1}X_n$ (M= Sc, Ti, V, Cr, Zr, Nb, Mo, Hf, Ta; X= C, N) with n = 1, 2, 3 that have recently been synthesized through hydrofluoric etching [2, 3] of layered MAX phase compounds $M_{n+1}AX_n$, where A = Al, Si, P, S, Ga, Ge, As, In, and Sn [4, 5]. During the etching process, the A element is washed out from the MAX phase structure and simultaneously the surfaces of the resulting 2D systems are chemically saturated with mixture of F, O, and OH [2, 3, 5, 6]. These 2D systems have been called Mxenes. The 2D MXenes such as Ti_2C, V_2C, Nb_2C, Ta_2C, Mo_2C, Ti_3C_2, Nb_4C_3 have already been synthesized [2, 3, 7].

Al- element containin MAX phases have been reported by Anasori and Dahlqvist [8-9] such as Mo_2TiAlC_2 and $Mo_2Ti_2AlC_3$. Furthermore, very recently Mo_2ScAlC_2 was synthesized by heating the mixture of elemental powders of Mo, Sc, Al and graphite at 1700°C [10]. Also MXene Mo_2ScC_2 was sytnhesized from MAX phase Mo_2ScAlC_2 [10]. In the present study, we aim to explore the structural and mechanical properties of new MXene of Mo_2ScC_2.

2.METHOD

First-principles calculations were performed using the augmented plane-wave pseudopotential approach to the density functional theory (DFT) implemented in Vienna Ab-initio Simulation Package (VASP)[13-15] We use the exchange-correlation potential within the Generalized Gradient Approximation (GGA) of Perdew, Burke, and Ernzerhof [17].The wave functions are expanded in the plane waves up to a kinetic-energy cutoff of 600 eV. The k-point is sampled according to the Monkhorst–Pack scheme[16], which yields 27 × 27 × 1 k-points, in the irreducible edge of Brillouin zone. The total energy is converged numerically to less than 1.10^{-6} eV/unit. After structural optimization, calculated forces are converged to less than 0.0001 eV/Å.

3. RESULTS AND DISCUSSION

MXenes obtain to from the MAX phases by removing A elements [2, 3]. Mo_2ScAlC_2 is hexagonal lattice structure. Firstly, we removed Al atoms from the Mo_2ScAlC_2 . The 2D structure of Mo_2ScC_2 monolayer was constructed by removing the Al atoms from the parent Mo_2ScAlC_2 phase.

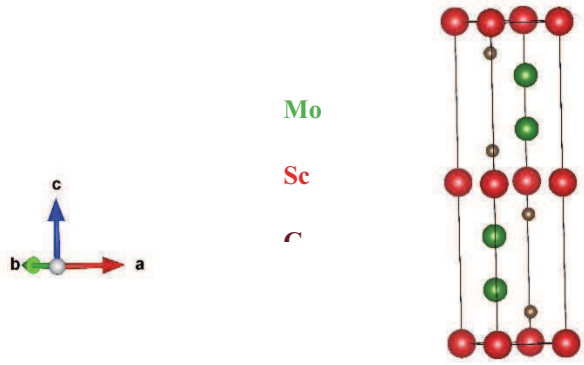

Figure 1. Unit Cell of Bulk Mo_2ScC_2

After this stage, we have optimized the Mo_2ScC_2 bulk structure. The result is listed below.

Table 1. The calculated lattice parameters (a, c in Å), ground state energy (E_0 in eV/fu), and volume (V_0 in $Å^3$/fu) with available experimental values.

Material	Space Group	a	c	V_0	E_0	Reference
Mo_2ScC_2(Bulk)	$P6_3/mcm$	3.16	14.86	129.17	-99.4	Present
Mo_2ScAlC_2	$P6_3/mcm$	3.03	18.77	149.61	-	Ref. [11]

In order to obtain Mo_2ScC_2 monolayer we constructed 1x1x3 supercell (the c direction) and removed excess atoms.

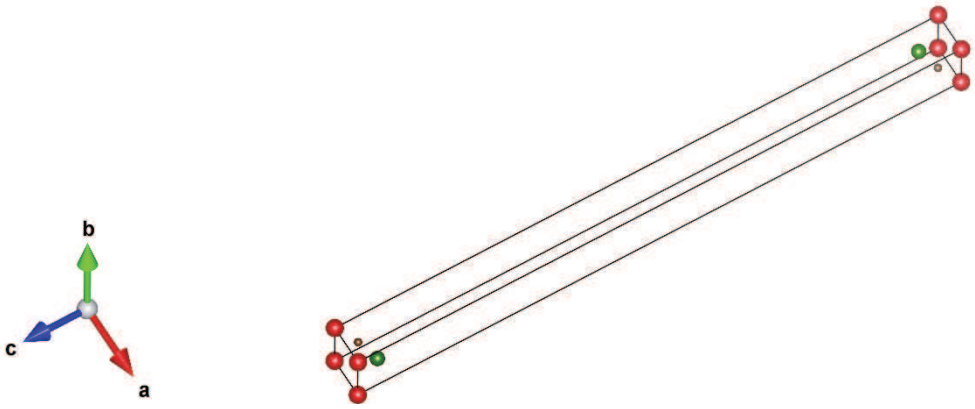

Figure 2. The Mo_2ScC_2 Monolayer

To prevent spurious interaction between isolated layers, a vacuum spacing of at least 35 Angstrom is introduced. Finally, we optimized this structure. so we were able to achieve a stable structure.

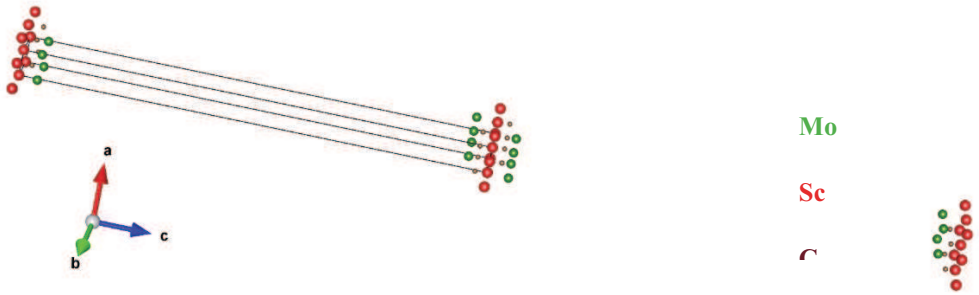

Figure 3. 2x2x2 Supercell of Mo_2ScC_2 Monolayer

2D Mo_2ScC_2 monolayer consists of a monatomic hexagonal plane between two monatomic hexagonal planes and forms a Mo–C–Sc-C-Mo sandwich structure.

Mechanical stability of 2D hexagonal crystals are tested according to Born criteria [18,19]. The following conditions have to be met for the mechanically stable.

$$C_{11} > 0,\ C_{44} > 0,\ 2*C_{44} = C_{11}-C_{12},\ C_{11} > |C_{12}|$$

4. CONCLUSION

In conclusion, we have studied the structural and mechanical properties of graphene-like hexagonal Mo_2ScC_2 monolayer using first-principles calculations within the generalized gradient approximation. We how that the Mo2ScC2 (double ordered Mxene) is structurally stable and indeed Mo_2ScC_2 has already been sytnhesized experimentally.

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REFERENCES

[1]. M. W. Barsoum, Prog. Solid State Chem. 28 (2001) 201.
[2] M. Naguib, M. Kurtoglu, V. Presser, J. Lu, J. Niu, M. Heon, L. Hultman, Y. Gogotsi, and M. W. Barsoum, Adv. Mater. 23, 4248 (2011).
[3] M. Naguib, O. Mashtalir, J. Carle, V. Presser, J. Lu, L. Hultman, Y. Gogotsi, and M. W. Barsoum, ACS Nano 6, 1322 (2012).
[4] M. Khazaei, M. Arai, T. Sasaki, M. Estili, and Y. Sakka, J. Phys.: Condens. Matter 26, 505503 (2014).
[5] M. Khazaei, M. Arai, T. Sasaki, M. Estili, and Y. Sakka, Sci. Tech. Adv. Mater. 15, 014208 (2014).
[6] M. A. Hope, A. C. Forse, K. J. Griffith, M. Lukatskaya, M. Chidiu, Y. Gogotsi, and C. P. Grey, Phys. Chem. Chem. Phys. 18, 5099 (2016).
[7] K. J. Harris, M. Bugnet, M. Naguib, M. W. Barsoum, and G. R. Goward, J. Phys. Chem. C 119, 13713 (2015).
[9] B.Anasori, M.R. Lukatskaya, Y.Gogotsi, Nature Rewiews Materiasl, 2017,16098.
[10] B.Anasori, M. Dahlqvist, J. Halim, E.J. Moon, J. Lu, B. C. Hosler, E. a. N. Caspi, S.J. May, L. Hultman, P. Eklund, J. Rosen, M. W. Barsoum, J. Appl. Phys. 118, 2015, 094304 - 094314.
[11] R. Meshkian, Q. Tao, M. Dahlqvist, J. Lu, L. Hultman and J. Rosen, Acta Materilia, 2017, 125, 476-480.
[12] M. Naguib, M. Kurtoglu, V. Presser, J. Lu, J. Niu, M. Heon, L. Hultman, Y. Gogotsi, M.W. Barsoum, Adv. Mater. 23 (2011) 4248.
[13] G. Kresse, J. Hafner, Phys. Rev. B 47 (1993) 558.
[14] G. Kresse, J. Furthmuller, Comput. Mater. Sci. 6 (1996) 15.
[15] G. Kresse, J. Furthmuller, Phys. Rev. B 54 (1996) 11169.
[16] H.J. Monkhorst, J.D. Pack, Phys. Rev. B 13 (1976) 5390.
[17] John P. Perdew, Kieron Burke, Matthias Ernzerhof, Phys. Rev. Lett. 77 (1996) 38.
[18] Mouhat F and Coudert F X 2014 Phys. Rev. B 90, 221104
[19] Nye J F 2012 Physical Properties oc Crystals: Their Represantation by Tensor and Mechanics (Oxford: Oxford University Press)