**Structure exploration for AB2 type monolayers**

**by high-throughput DFT calculations**

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Two-dimensional (2D) monolayers have attracted incredible interest because of their peculiarities and novel properties. For example, graphene and silicene are well known as atomically thin monolayers. Boron nitride and silicon carbide are known as AB type monolayers. In addition, various kinds of monolayers of transion metal (A=Mo, W, etc.) dichalcogenides (B=S, Se or Te) with a formula AB2, which are arranged in triatomic layers, have been recently synthesized experimentally for producing a AB2 type 2D transition metal chalcogenide library [1]. These kinds of investigations have revealed interesting phenomena such as two-demensional superconductivity and quantum spin Hall effect. However, it can be considered that several kinds of 2D structures which can exist stably may have not been synthesized experimentally yet since the combination of the elements is diverse even only for the AB2 composition. Therefore, there is a room for exploring unknown monolayers.

In this study, we performed high-throughput calculations based on the density functional theory by using OpenMX[2] to create a structure map for AB2 type monolayers. At first, we categorized the AB2 structures into planar, 1T (trigonal) phase (ex. ZrS2 [1]), 2H (hexagonal) phase (ex. MoS2 [1]), memory structure and the others. Here, the group of “planar” means B atoms form almost honeycomb structures and A atoms are on the center of the honeycombs. The group of “memory structure” means that the structure is similar to the planar, but A atoms are shifted from the plane formed by B atoms. Since the positions (up or down) of A atoms can represent binary digits, we call the backled structures “memory structure” here. This structure can be a candidate for a data strage application with an extremely high areal density. Next, we prepared 2×2 supercell AB2 initial structures (1T, 2H and planar) for selected compounds (62 elements×62 elements=3844 compounds), where compounds of noble gases, lanthanides and actinides are excluded. After geometry relaxations and variable cell optimizations were carried out, the most stable converged structures were summarized on the structure map for AB2 type monolayers.

From the structure map, we predicted that some of the structures can be the memory structure. Some NEB calculations for these memory structures indicate that it may be possible to control them as binary digits strage applications. In this presentation, we report the details of the high-throughput calculations and show some obtained interesting structures.

[1] J. Zhou *et al.*, Nature **556**, 355 (2018)

[2] OpenMX, http://www.openmx-square.org/.

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