Two-dimensional structures for non-layered materials

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Two-dimensional (2D) materials have been studied extensively due to their intriguing properties and potential applications. 2D materials are usually exfoliated from layered materials that consist of atomically thin layers vertically stacked via van der Waals (vdW) forces. On the other hand, 2D materials created from non-layered materials have also been synthesized experimentally.

In this project, we have studied non-vdW 2D materials using Quantum ESPRESSO package. First, we investigated the structural properties of 2D strontium titanate ($SrTiO_3$) [see Fig. 1(a)] [1]. This is constructed by stacking SrO, TiO_2, and SrO monolayers, and the chemical formula is Sr_2TiO_4. We have shown that the TiO_6 octahedral rotations emerge with a rotation angle twice that in the 3D bulk. The rotation angle decreases when the film thickness is increased. Using the molecular dynamics (MD) simulation, we have demonstrated that the cubic-like phase appears above 1000 K [see Fig. 1(b) and 1(c)]. Such a phase transition temperature is higher than of 3D bulk. The effect of octahedral rotations on the electronic properties is also discussed.

We have also explored fluorite-type (CaF_2-type) materials in the 2D limit [2]. The crystal structures of fluorite-type materials are extracted by using Materials Project database and pymatgen code. More than 30 monolayers truncated from the surface have negative formation energy and they are dynamically stable. In addition, several monolayers are identified to exhibit negative Poisson's ratio. The present work has provided novel non-vdW materials in the 2D limit.

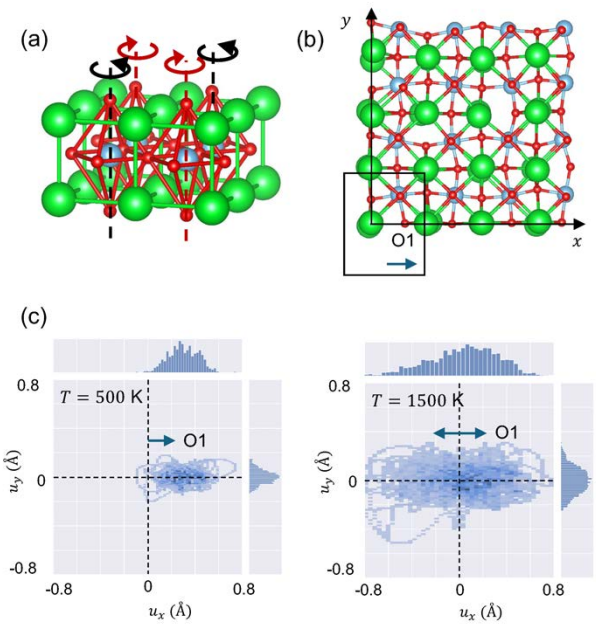

Figure 1: (a) 2D $SrTiO_3$ monolayer. The TiO_6 octahedra are elongated along the out-of-plane direction and rotate around the z axis. (b) Atomic distribution of 2D $SrTiO_3$ monolayer after a MD simulation of 5 ps for 500 K. The O1 atom shifts in the x direction. (c) The displacement distribution of O1 atom within the x-y plane at 500 K (left) and 1500 K (right).

References

[1] S. Ono and Y. Kumagai: J. Phys. Soc. Jpn. **92**, 114601 (2023).

[2] S. Ono and R. Pawar: *in preparation.*