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Exploitable magnetic anisotropy of magnetic $CrBr_3$ monolayer

M. Luo[+1)], *Y. H. Shen*[*]

[+]*Department of Physics, Shanghai Polytechnic University, 201209 Shanghai, China*

[*]*Key Laboratory of Polar Materials and Devices, East China Normal University, 200241 Shanghai, China*

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Magnetic anisotropy energy (MAE) plays a key role in two dimensional (2D) magnetic materials, and it could overcome the thermal fluctuations and stabilizes the magnetic order at the finite temperature which has been verified by the Mermin–Wagner theorem. Moreover, ferromagnetic 2D materials with large anisotropy comes attract growing attention for their potential applications in spintronic devices. It is considerably attractive to explore whether intrinsic ferromagnetism and the magnetic anisotropy of 2D monolayer can be modulated. Previous works indicated that surface adsorption is an attractive approach to control electronic structure and magnetism in 2D materials. As we known, $CrBr_3$ and CrI_3 are intrinsic magnetic materials. Many works have been carried out to investigate the MAE in these materials. However, the study of how to control MAE of $CrBr_3$ is still lack. In this work, the impact of Li and F adsorptions on the electronic and magnetic properties of monolayer $CrBr_3$ are investigated by first-principles calculations, as shown in Fig. 1a. It is observed that Li adsorption can dramatically enhance its ferromagnetism, but the ferromagnetism is reduced by the F adsorption, as shown in Fig. 1b. Interestingly, the easy magnetization axis switches from original out-of-plane to in-plane direction. As shown in Fig. 1c, we find that the easy axis of monolayer $CrBr_3$ can be tuned from the out-of-plane to in-plane after Li adsorption. By contrast, as shown in Fig. 1d, while the monolayer $CrBr_3$ is adsorbed by F, the easy axis maintains out-of-plane. Our study illustrates the promising potential of electrostatic doping induced by charge transfer in tuning the magnetization orientation and enhancing ferromagnetism in monolayer $CrBr_3$.

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[1)]e-mail: mluo@gench.edu.cn

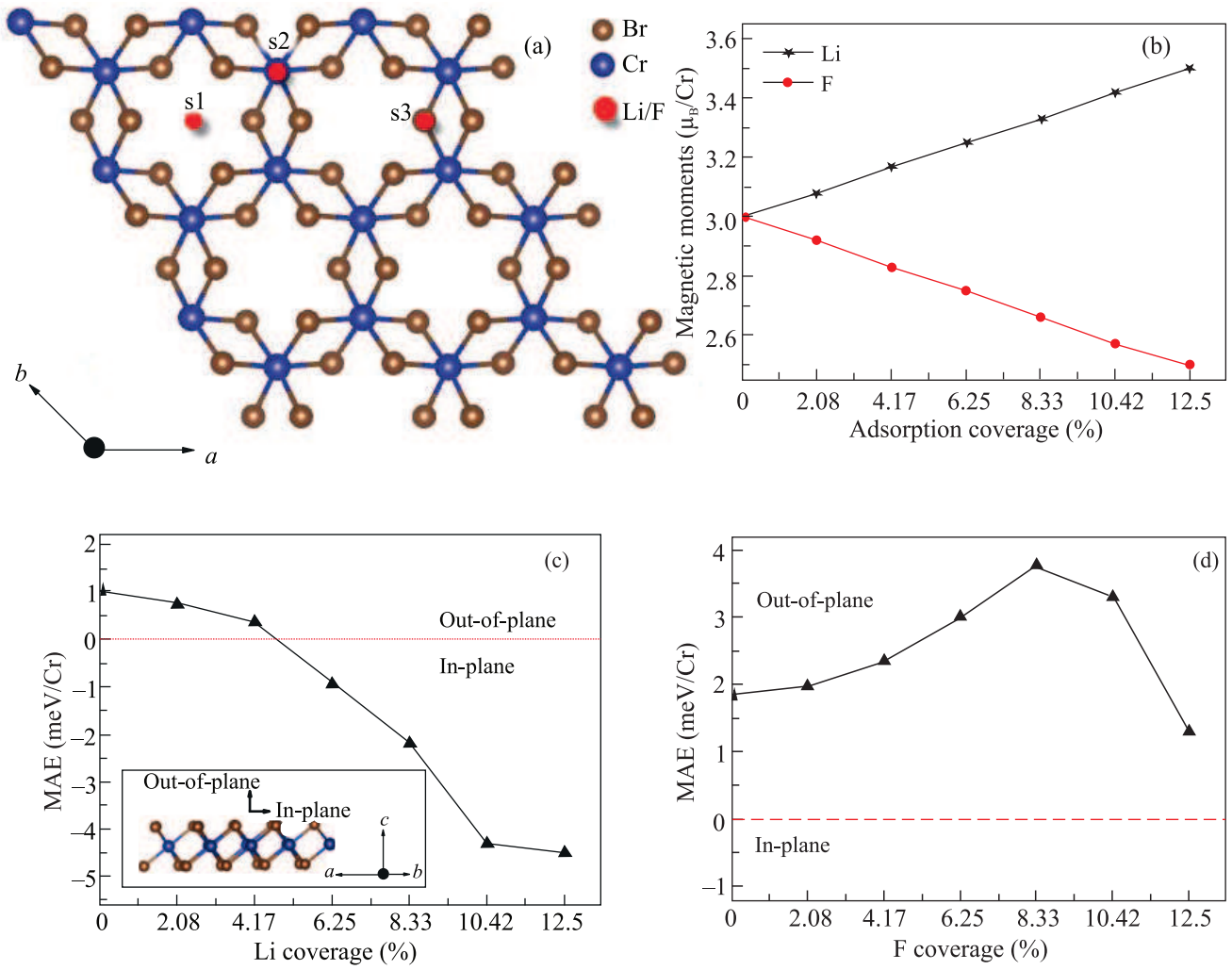

Fig. 1. (Color online) (a) – Top view of pristine $CrBr_3$ monolayer and three possible adsorption sties of Li (F) are marked. s1 – Hollow, s2 – Cr-top, s3 – Br-top. (b) – The local magnetic moment of Cr in the Li- and F-adsorbed $3 \times 2 \times 1$ $CrBr_3$ monolayer; Magnetic anisotropy energy (MAE) of the $CrBr_3$ monolayer with different Li (c) and F (d) adsorption coverage

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