Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supplemental Material

Prediction of two-dimensional monolayer C_2O_2Fe with chiral magnetic and ferroelectric orders

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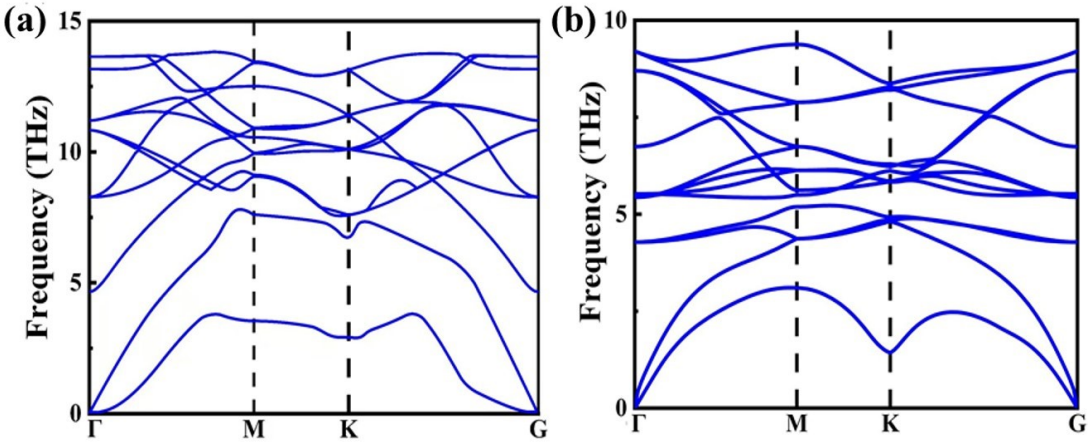

Fig.S1 Phonon dispersion of C_2O_2Fe monolayer at (a) 0% strain and (b) 30% strain, where all acoustic branch frequencies are positive, indicating its dynamic stability. Meanwhile, the highest optical frequency at no strain is higher than that at 30% one, suggesting the stronger bonding nature at no strain.

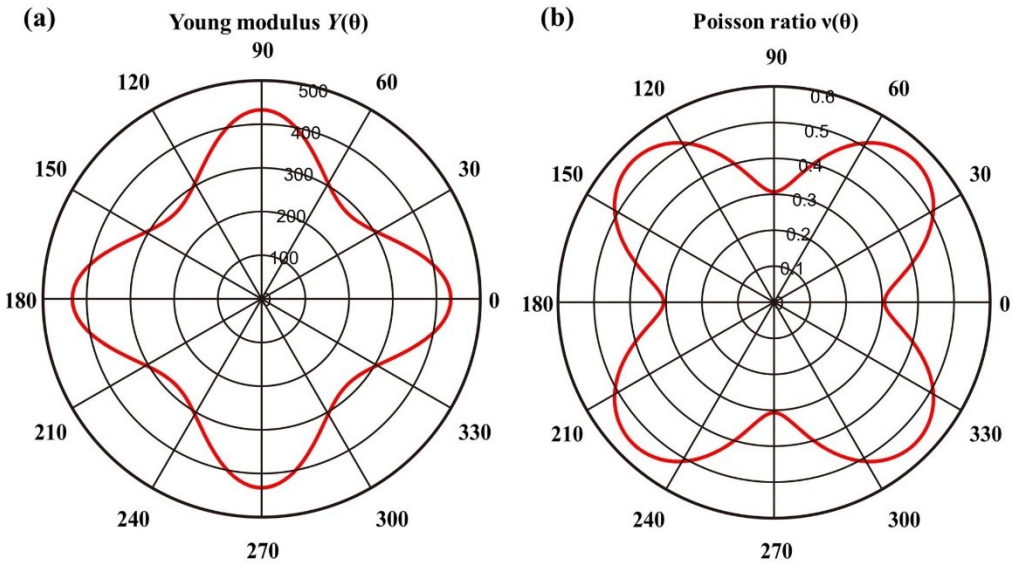

Fig.S2 In-plane (a) Young's modulus, (b) Poisson's ratio for C_2O_2Fe monolayer with 30% strain, where we find that Young's modulus and Poisson's ratios of C_2O_2Fe monolayer change from 289.32 N/m^2 and 0.56 at $\theta = 45^o$ to 432.68 N/m^2 and 0.31 at $\theta = 90^o$. The maximum value of Young's modulus is less than these of many other 2D materials.[1] For Poisson's ratio, it is consistent to most of the 2D materials (0−0.5).[2]

References

1 Z. Gao, X. Dong, N. Li, J. Ren, *Nano Lett.*, 2017, **17**, 772-777.

2 D. W. Boukhvalov, M. I. Katsnelson, *J. Am. Chem. Soc.*, 2008, **130**, 10697-10701.