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**Exploring the low friction of diamond-like carbon films in carbon dioxide atmosphere  
by experiments and first-principles calculations**

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### Graphical Abstract

The experiments demonstrate that DLC films in CO<sub>2</sub> atmosphere exhibit low friction coefficient compared with in ambient air and vacuum atmospheres (Fig.1a). The results of first-principle calculation reveal that the lactone groups can easily form during the horizontally chemisorption of CO<sub>2</sub> molecule on the DLC surface during the shearing sliding, which means that the “dangling bonds” of the DLC surface are passivated by the activated CO<sub>2</sub>. (Fig.1b). The resulting lactone group is the main cause of the low friction behavior of

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