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Tuning frictions between graphene layers via Li ion intercalation[1]
AIJIANG LU, Donghua University, JIAYU WAN, TENG LI, LIANGBING HU, Univ of Maryland-College Park, UNIVERISYT OF MARYLAND, COLLEGE PARK TEAM — Graphite intercalated with Li ions are widely studied and applied in Li ion batteries. It was revealed in experiments that, the Li ion intercalation leads to a phase transition of the graphite with about 10% volume expansion. The increased interlayer distance should contribute to decrease the frictions between the grahene layers, but the Li ion intercalation would take an opposite effect. In order to show the total effect of the Li ion interalation, we studied the frictions between graphene layers with and without lithiation, based on density functional theory (DFT). In a sandwich-like model, slipping of the middle sheet of the graphene was simulated. Displacements between layers were fixed and the other parts were relaxed, thus the energies were record to estimate the energy barriers accordingly. We found that the frictions between the graphene layers with the Li ion intercalation are higher than those without intercalation. The energy barrier appears correlated with the concentration of the intercalated ions. As the atomic ratio between lithium and carbon increases from 0 (no intercalation) to 1:6, the energy barriers increase from 0.01 eV/atom to 0.05 eV/atom or so. Such an interesting result indicates that, just via ion intercalation, we can effectively tune the friction between graphene layers.

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Jiayu Wan
Univ of Maryland-College Park

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