Phase changing in graphite by interface charge injection

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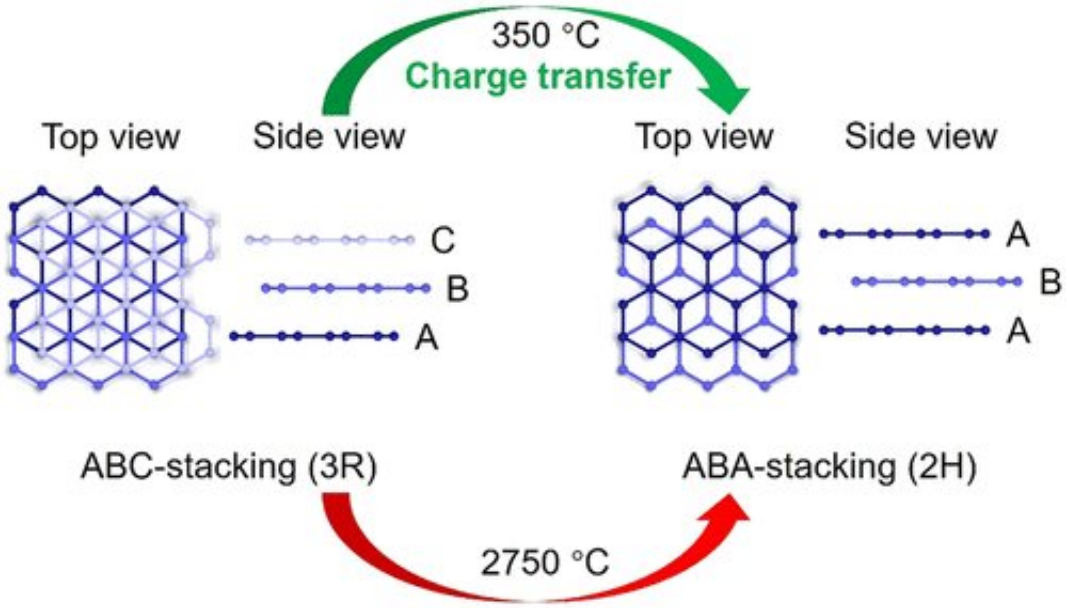

The charge transfer from α-Li3N to graphite can lower the transition temperature down to 350 degrees C. Credit: PAN Fei et al.

Graphite, as an important material for Li battery anode and graphene preparation, can exist in two phases: the Bernal (2H) phase and the rhombohedral (3R) phase. The 2H phase has relatively low energy and high proportion in graphite powder, while the 3R phase shows the opposite properties. However, the decrease of the flake graphite size gives rise to the proportion of 3R phase up to 50%.

According to existed researches of graphite phase changing, the transition from 3R phase to 2H phase is usually observed under high temperature over 1,000 degrees C through Joule or laser heating, which is inappropriate and unfeasible.

A research team led by Prof. ZHU Yanwu from University of Science and Technology of China (USTC) of the Chinese Academy of Sciences (CAS) has achieved full conversion of 3R to 2H at about 350 degrees C by annealing graphite in the presence of α-Li3N (lithium nitride), a promising material for catalysis and energy applications.

Based on this, the team revealed the mechanism of reduction of the energy barrier in the presence of α-Li3N collaborating with researchers from the National University of Defense Technology, the Northwestern Polytechnical University, the Institute of Semiconductors of CAS, and the University of Manchester. The study was published in *Nano Letters*.

An interface charge injection from α-Li3N to the conjugated π bond of graphite enlarged interlayer distance. This made the layer slipping occur more easily, allowing a lower phase transition temperature from 3R to 2H in graphite.

To explore the interlayer slipping pathway during the phase transition from 3R to 2H, the researchers employed the in-situ X-ray diffraction analysis and the density functional theory calculations. Moreover, Raman mapping was performed on mechanically exfoliated graphite flakes before and after the introduction of α-Li3N particles, further confirming the doping caused by α-Li_3N.

These results provide a possible way to control the stacking configuration and other properties of graphite through regulating the conjugated π bond, also making it attractive for future carbon material preparation.

More information: Fei Pan et al, Phase-Changing in Graphite Assisted by Interface Charge Injection, *Nano Letters* (2021). DOI: 10.1021/acs.nanolett.1c01225