# Compressive behaviors of porous graphene aerogel and its application in high performance supercapacitor

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## Abstract

Ultralight and compressible carbon materials have promising application in energy storage devices. Graphene aerogel (GA) is a free-standing three-dimensional framework constructed by interconnected graphene sheets and the honeycomb-like porous network endows GA with good compressibility and high specific surface, especially suitable for high performance supercapacitor electrode materials.

In this work, the compressive behaviors of honeycomb-like GA is investigated via the molecular dynamics (MD) simulations via adaptive intermolecular reactive empirical bond order (AIREBO) potential. The effects of layer number, size of graphene sheet, interlayer crosslink density and loading rate on the compressive behaviors of GA have been systematically studied. The two main deformation patterns are presented under different loading rate. Moreover, the nitrogen and sulfur co-doped GA (N,S-GA) was experimentally prepared in one-step process, where the porous structure provides electrically conductive channels for electrolyte and heteroatoms transfer to improve the chemical reactivity and electronic property of the GA electrodes. The optimized N,S-GA, as a bind-free electrode for supercapacitor, exhibits a high specific capacitance (323.8 F $g^{-1}$ at 1A $g^{-1}$), long cycle life (91.6% retention of the initial capacitance over 10,000 cycles) and excellent rate capability. The capacitance is about twice larger than that of pure GA because of the synergistic effect of N and S, which agrees well with the calculation of absorption energy of N,S-GA with electrolyte. Therefore, the large capacitance for the optimized N,S-GA is attributed to the fast ion diffusion, large accessible area (porous network) and increased pseudocapacitance (N and S).

Considering the advantages of the facile strategy for synthesizing N,S-GA with honeycomb-like network and the low cost of the raw materials, the N,S-GA electrodes show more opportunities for the fabrication of a variety of energy storage applications.

**Keywords:** Compressive behaviors, Graphene aerogel, Hierarchical porous network, Supercapacitor.