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A first-principles study on Magnetic and Electronic properties of Graphane vacancies Dots. BI-RU WU, Department of Natural science, Center for General Education, Chang Gung University, Kueishan 333, CHIH-KAI YANG, Graduate Institute of Applied Physics, National Chengchi University,Taipei 11605 — Graphane is the end product of the complete hydrogenation of graphene. The incomplete hydrogenation of graphene produces hydrogen vacancies in graphane. Hydrogen vacancies can alter the electronic structure of graphane and therefore tune the electronic, magnetic, and optical properties of the composite. In this paper, we use a first-principles density functional calculation to investigate a variety of well-separated clusters of hydrogen vacancies in graphane with magnetism, including the geometrical shapes of triangles, parallelograms, and rectangles. The results indicate that energy levels caused by the missing H are generated in the broad band gap of pure graphane. All triangular clusters of H vacancies are magnetic, the larger the triangle the higher the magnetic moment. The defect levels introduced by the missing H in triangular and parallelogram clusters are spin-polarized and can find application in optical transition. Parallelograms and open-ended rectangles are antiferromagnetic and can be used for nanoscale registration of digital information.

Bi-Ru Wu
Department of Natural science, Center for General Education, Chang Gung University

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