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A first-principles investigation on the Electronic and Magnetic properties of Hydrogen vacancy chains in Graphane BI RU WU, Department of Natural science, Center for General Education, Chang Gung University, CHIH-KAI YANG, Graduate Institute of Applied Physics, National Chengchi University — We investigated a variety of configurations of hydrogen-vacancy (HV) chains in graphane with density functional theory. We found the configurations that each of zigzagged HV chains separated by one or more H chains exhibit nonmagnetic conductor or has a tiny gap. Once as the neighbored zigzag HV chains blocked by isolated H atoms, the structure transformed from a nonmagnetic conductor into a magnetic semiconductor. If the HV chains are continuously distributed, it looks like a graphene nanoribbon embedded in graphane. The zigzag edged embedded graphene nanoribbons also show antiferromagnetic. An additional H atom on the ribbon can tune the band gap and generate magnetic moment; moreover, if bare C atoms are present outside the nanoribbon also have similar effect. The results will be helpful for designing graphene-based nanoelectronic devices.

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