Abstract Submitted
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Magnetization of Graphane by Dehydrogenation[1] HASAN SAHIN, Bilkent University, UNAM-Institute of Material Science and Nanotechnology, CAN ATACA, Bilkent University, SALIM CIRACI, Bilkent University, UNAM-Institute of Material Science and Nanotechnology — Using first principles calculations, we show that each hydrogen vacancy created at graphane surface results in a local unpaired spin. For domains of hydrogen vacancies the situation is, however complex and depends on the size and geometry of domains, as well as whether the domains are single- or double-sided. In single-sided domains, hydrogen atoms at the other side are relocated to pair the spins of adjacent carbon atoms by forming π-bonds. Owing to the different characters of exchange coupling in different ranges and interplay between unpaired spin and the binding geometry of hydrogen, vacancy domains can attain sizable net magnetic moments.

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Hasan Sahin
Bilkent University, UNAM-Institute of
Material Science and Nanotechnology

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